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|  |  |   |   |
|--|--|---|---|
| (51) Internationale Patentklassifikation <sup>6</sup> :<br><b>C07D 235/20, A61K 31/485, C07D 211/58, A61K 31/445, C07D 279/18, A61K 31/155, C07C 237/10, A61K 31/16, C07D 213/44, 213/82</b>   |  | A2  | (11) Internationale Veröffentlichungsnummer: <b>WO 99/40073</b> |
|  |  | (43) Internationales Veröffentlichungsdatum:  | 12. August 1999 (12.08.99)                                      |
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| (22) Internationales Anmeldedatum: <b>4. Februar 1999 (04.02.99)</b>   |  |   |   |
| (30) Prioritätsdaten:<br>198 04 761.4      6. Februar 1998 (06.02.98)      DE<br>198 51 300.3      6. November 1998 (06.11.98)      DE   |  |   |   |
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| (54) Title: <b>TRYPTASE INHIBITORS</b>   |  | Veröffentlicht<br>Ohne internationalen Recherchenbericht und erneut zu veröffentlichen nach Erhalt des Berichts.  |   |
| (54) Bezeichnung: <b>TRYPTASE-INHIBITOREN</b>  |  |   |   |
| <div style="display: flex; align-items: center; justify-content: center;"> <div style="text-align: center;"> <math display="block">\begin{array}{c} \diagup K1 \\ L \\ \diagdown K2 \end{array} \quad (I)</math> </div> <div style="margin: 0 20px;">(I)</div> <div style="text-align: center;"> <math display="block">\begin{array}{c} B1 - A1 - B3 - A3 - B5 - A5 - \\ B2 - A2 - B4 - A4 - B6 - A6 - \end{array} \quad (II)</math> </div> </div>   |  |   |   |
| (57) Abstract  |  |   |   |
| <p>The invention relates to bifunctional inhibitors of human tryptase of formula (I), to human tryptase in crystalline form, to a method for producing human tryptase in crystalline form, to pharmaceutical compositions comprising a bifunctional inhibitor of human tryptase, and to a method for developing and identifying tryptase inhibitors. The tryptase inhibitors are characterized in that both head groups K1 and K2 are the same or different and each comprises a group Q which can interact with a carboxylate group. The linker L can assume a conformation such that the groups Q of both head groups are situated at a distance ranging from 20 to 45 Å, such that the dimension of the head groups and of the linker permit the inhibitor to penetrate into a cavity with the dimensions 52 Å X 32 Å X 40 Å, and such that L represents formula (II) wherein A1 and A2 are the same or different, and represent -C(O)-, NH-, -O- (oxygen), -S- (sulfur), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- or a bond. A3 and A4 are the same or different and represent -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- or a bond, or are selected from the group A5, A6, M, B1-B6 as stated in the description.</p> |  |   |   |

### (57) Zusammenfassung

Die Erfindung betrifft bifunktionelle Inhibitoren von humaner Tryptase der Formel (I), humane Tryptase in kristallisierter Form, ein Verfahren zur Herstellung von humaner Tryptase in kristallisierter Form, pharmazeutische Zusammensetzungen, umfassend einen bifunktionellen Inhibitor von humaner Tryptase sowie ein Verfahren zur Entwicklung und Identifizierung von Tryptase-Inhibitoren, dadurch gekennzeichnet, dass die beiden Kopfgruppen K1 und K2 gleich oder verschieden sind und jeweils eine Gruppe Q umfassen, die mit einer Carboxylatgruppe Wechselwirkungen eingehen kann, der Linker L eine Konformation einnehmen kann, so daß die Gruppen Q der beiden Kopfgruppen in einem Abstand von 20 bis 45 Å vorliegen, die Ausmaße der Kopfgruppen und des Linkers das Eindringen des Inhibitors in einen Hohlraum mit den Dimensionen 52 Å x 32 Å x 40 Å erlauben, und L für die Formel (II) steht, worin A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten, A3 und A4 gleich verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe A5, A6, M, B1-B6 wie in der Beschreibung.

### LEDIGLICH ZUR INFORMATION

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## Tryptase-Inhibitoren

### Beschreibung

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Die Erfindung betrifft bifunktionelle Inhibitoren von humaner Tryptase, humane Tryptase in kristallisierter Form, ein Verfahren zur Herstellung von humaner Tryptase in kristallisierter Form, pharmazeutische Zusammensetzungen, umfassend einen bifunktionellen Inhibitor von humaner Tryptase sowie ein Verfahren zur Entwicklung und Identifizierung von Tryptase-Inhibitoren.

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Humane Tryptase ist eine Serinproteinase, die in humanen Mastzellen das überwiegend vorliegende Protein darstellt. Tryptase umfaßt vier eng verwandte Enzyme ( $\alpha$ , I, II/ $\beta$ , III; mit 90 bis 98 % Sequenzidentität) (vgl. Miller et al., J.Clin.Invest. 84 (1989) 1188-1195; Miller et al., J.Clin.Invest. 86 (1990) 864-870; Vanderslice et al., Proc.Natl.Acad.Sci., USA 87 (1990) 3811-3815). Mit Ausnahme der  $\alpha$ -Tryptase (Schwartz et al., J.Clin.Invest. 96 (1995) 2702-2710; Sakai et al., J.Clin.Invest. 97 (1996) 988-995) werden die Enzyme intrazellulär aktiviert und in katalytisch aktiver Form in Sekretgranulen gelagert.

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Tryptase weist im Vergleich zu anderen bekannten Serinproteinasen, wie z.B. Trypsin oder Chymotrypsin einige besondere Eigenschaften auf (Schwartz et al., Methods Enzymol. 244, (1994), 88-100; G.H. Caughey, "Mast cell proteases in immunology and biology." Marcel Dekker, Inc., New York, 1995). Tryptase aus humanem Gewebe weist eine nicht kovalent verknüpfte tetramere Struktur auf, die durch Heparin oder andere Proteoglycane stabilisiert sein muss, um proteolytisch aktiv zu sein.

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Weiterhin ist bis jetzt kein Faktor im Serum bekannt, der Tryptase hemmt. Es ist bis jetzt nicht gelungen, einen endogenen Inhibitor für Tryptase aufzufinden. Tryptase wird auch mit Ausnahme des atypischen Inhibitors LDTI (Leech Derived Tryptase Inhibitor) (Sommerhoff et al., Biol.Chem.Hoppe-Seyler 375 (1994) 685-694) nicht durch natürlich auftretende Proteinaseinhibitoren gehemmt.

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Weiterhin weist Tryptase eine unübliche, sehr enge Substratspezifität auf, wobei eine Reihe von Peptidsubstraten in vitro gespalten werden (Tam et al., Am.J.Respir.Cell Mol. Biol. 3 (1990) 27-32), aber nur wenige ausgewählte Proteine. Beispielsweise werden Fibrinogen, Fibronectin und hochmolekulares Kininogen inaktiviert (Schwartz et al., J.Immunol., 135(4) (1985), 2762-2767; Lohi et al., J. Cell. Biochem. 50, (1992), 337-349; Little et al., Biochem. J. 307 (1995) 341-346) und die Zymogene von Stromelysin (proMMP-3) und der Plasminogenaktivator des Urokinasetyps (pro-uPA) aktiviert (Gruber et al., J. Clin. Invest. 84 (1989), 1657-1662; Lees et

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al., Eur. J. Biochem. 223 (1994), 171-177; Stack et al., J. Biol. Chem. 269 (1994), 9416-9419). Weiterhin wurde festgestellt, dass Tryptase mitogene Wirkungen zeigt (Ruoss et al., J. Clin. Invest. 88 (1991), 493-499; Hartmann et al., Am. J. Physiol. 262 (1992), L528-L534; Brown et al., Am. J. Respir. Cell Mol. Biol. 13 (1995), 227-236).

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Tryptase wird zusammen mit anderen Entzündungsmediatoren, wie z.B. Histamin und Proteoglycanen, freigesetzt, wenn humane Mastzellen aktiviert werden. Man vermutet deshalb, dass Tryptase bei einer Reihe von Erkrankungen, insbesondere bei allergischen und entzündlichen Erkrankungen eine Rolle spielt, zum einen aufgrund der Bedeutung von Mastzellen bei solchen Erkrankungen und zum anderen, da bei einer Reihe derartiger Erkrankungen ein erhöhter Tryptase-Gehalt festgestellt wurde. So wird Tryptase u.a. mit folgenden Erkrankungen in Zusammenhang gebracht: Akute und chronische (insbesondere entzündliche und allergen induzierte) Atemwegserkrankungen verschiedener Genese ( z. B. Bronchitis, allergische Bronchitis, Asthma bronchiale, COPD); interstitielle Lungenerkrankungen; Erkrankungen, die auf allergischen Reaktionen der oberen Atemwege (Rachenraum, Nase) und der angrenzenden Regionen (z. B. Nasennebenhöhlen, Augenbindehäute) beruhen, wie beispielsweise allergische Konjunktivitis und allergische Rhinitis; Erkrankungen aus dem Formenkreis der Arthritis (z. B. rheumatische Arthritis); Autoimmun-Erkrankungen wie Multiple Sklerose; desweiteren Periodontitis, Anaphylaxis, interstitiale Cystitis, Dermatitis, Psoriasis, Sklerodermie/systemische Sklerose, entzündliche Darmerkrankungen (Morbus Crohn, Inflammatory Bowel Disease) und andere. Tryptase scheint insbesondere direkt mit der Pathogenese von Asthma in Zusammenhang zu stehen (Caughey, Am. J. Respir. Cell Mol. Biol. 16 (1997), 621-628; R. Tanaka, „The role of tryptase in allergic inflammation“ in: Protease Inhibitors, IBC Library Series, 1979, Kapitel 3.3.1-3.3.23).

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Zur genauen Untersuchung der Funktion von Tryptase, insbesondere bei allergischen und entzündlichen Erkrankungen, ist jedoch die Entwicklung von selektiven Tryptase-Inhibitoren notwendig. Bisher wurden Tryptase-Inhibitoren auf Grundlage der dem Trypsin ähnlichen Aktivität und Spezifität von Tryptase entworfen und synthetisiert, wobei zumeist von einer Benzamidingruppe als Substratrest ausgegangen worden ist. Mehr oder weniger gute Inhibitoren wurden durch die Methode "trial and error" gefunden, wobei insbesondere Benzamidin- und ähnliche Strukturen mit mehr oder weniger starren und hydrophoben Gruppen derivatisiert wurden. Ein Beispiel hierfür ist 4-Amidinophenylbrenztraubensäure (APPA, Amidinophenyl pyruvic acid; Stürzebecher et al., Biol. Chem. Hoppe-Seyler 373 (1992), 1025-1030). Solche Inhibitoren auf Benzamidinbasis sind jedoch nicht selektiv für Tryptase, sondern hemmen auch andere physiologisch wichtige Enzyme, wie beispielsweise Thrombin, Faktor Xa und Urokinase. Sie sind deshalb nicht zur selektiven Untersuchung der Funktion von Tryptase verwendbar.

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- Weiterhin wurde im Stand der Technik ein peptidischer Tryptaseinhibitor, nämlich N-(1-Hydroxy-2-naphthoyl)-L-arginyl-L-prolinamid, beschrieben (R. Tanaka, *Protease Inhibitors*, IBC Series 1997, Kapitel 3.3; Clark et al., *Drugs of the future* 21 (8) (1996), 811-816; WO 94/20527).
- 5 Auch dieser Inhibitor ist jedoch nicht selektiv für Tryptase, sondern hemmt auch andere Proteinasen wie etwa Trypsin und Thrombin, sodass nicht eindeutig festgestellt werden kann, ob beobachtete Wirkungen aufgrund einer spezifischen Hemmung von Tryptase erzielt werden oder vielmehr durch andere Vorgänge.
- 10 Ein weiterer im Stand der Technik beschriebener Tryptaseinhibitor ist LDTI, ein Inhibitor vom Kazal-Typ, der aus Blutegeln isoliert wurde (LDTI, leech-derived tryptase inhibitor) (WO95/03333; Stubbs et al., *J. Biol. Chem.* 272 (32) (1979), 19931-19937; WO97/22626). Es handelt sich um einen proteinartigen Inhibitor, dessen Struktur anhand von NMR-Daten und von LDTI-, Trypsin-Kristallen bestimmt wurde. Dabei wurde festgestellt, dass der basische
- 15 Aminoterminus von LDTI vermutlich einen elektrostatischen Beitrag zur Wechselwirkung mit Tryptase liefert. Bei LDTI handelt es sich zwar um einen Inhibitor mit hoher Affinität zu Tryptase ( $K_i$  von 1,4 nM), LDTI inhibiert aber auch Trypsin und Chymotrypsin im nanomolaren Bereich.

- Als weiterer Inhibitor von Tryptase wurde SLPI (Sekretory leucocyte protease inhibitor)
- 20 vorgeschlagen (WO96/08275 A1). Auch hierbei handelt es sich um einen proteinartigen Inhibitor. WO95/32945, WO96/09297 und WO98/04537 schließlich beschreiben niedermolekulare Verbindungen als Tryptaseinhibitoren. Diese Verbindungen weisen an den Enden überwiegend Amino, Guanidino oder Amidinogruppen auf. Die Wirksamkeit dieser Verbindungen wird ebenfalls durch "trial and error" bestimmt.

- 25 Eine Aufgabe der vorliegenden Erfindung war es deshalb, hochspezifische Inhibitoren von humaner Tryptase bereitzustellen, deren Wirksamkeit anhand struktureller Parameter zuverlässig vorausgesagt werden kann. Diese Aufgabe wird erfindungsgemäß gelöst durch einen bifunktionellen Inhibitor von humaner Tryptase, der dadurch gekennzeichnet ist, dass er
- 30 zwei Kopfgruppen K1 und K2 umfasst, die durch einen Linker L verbunden sind, wobei K1 und K2 gleich oder verschieden sind und jeweils eine Gruppe Q umfassen, die mit einer Carboxylatgruppe Wechselwirkungen eingehen kann, wobei der Linker L eine solche Konformation einnehmen kann, dass die Gruppen Q der beiden Kopfgruppen in einem Abstand von 20 bis 45 Å vorliegen, und wobei die Ausmaße der Kopfgruppen und des Linkers das Eindringen des
- 35 Inhibitors in einen Hohlraum mit den Dimensionen 52 Å x 32 Å x 40 Å erlauben. Ausführungsformen der Gruppe Q werden hierin auch als Gruppe X1, X2 bzw. Gruppe Y1, Y2 bezeichnet und werden nachfolgend näher definiert.

Es ist überraschenderweise gelungen, Kristalle von humaner  $\beta$ -Tryptase aus Mastzellen zu erhalten und eine Röntgenkristallstrukturanalyse durchzuführen. Diese hat eine exakte Bestimmung der räumlichen dreidimensionalen Geometrie des Tryptase-Tetramers ermöglicht, wodurch wichtige Erkenntnisse im Hinblick auf die Entwicklung von Tryptase-Inhibitoren erhalten wurden.

Es wurde gefunden, dass in den Kristallen flache, quadratische, rahmenartige Tetramere mit den Dimensionen  $82 \times 80 \times 40 \text{ \AA}$  aufeinander entlang einer  $4_1$ -Schraubenachse gestapelt sind. Entlang seiner vier Kanten befindet sich jedes Tetramer in engem Kontakt mit Symmetrieverwandten Nachbarn, sodass sich ausgedehnte Schichten bilden. Innerhalb eines Tetramers befindet sich eine Tryptaseeinheit an jeder Ecke des Tetramers, d.h. jedes der vier, chemisch identischen Monomeren besetzt eine Ecke des flachen Rahmens mit nahezu quadratischer Gestalt. Die vier Tryptaseeinheiten des Tetramers begrenzen einen zentralen, ovalen Kanal bzw. eine zentrale Pore mit den ungefähren Ausmaßen  $52 \times 32 \times 40$  (Tiefe)  $\text{\AA}$ . Die beiden Eingänge zu dieser Pore sind teilweise durch eine von jedem der Monomeren vorspringende Peptidschleife verstellt (147er-Schleife). Dies bewirkt, dass sich die Pore im Inneren zu einer größeren Höhle erweitert.

Die gefundene flache, rahmenförmige Struktur des Tryptasetetramers ist überraschend und unterscheidet sich grundsätzlich von den bisher veröffentlichten schematischen Tryptasemodellen, in denen eine kompakte, "quasi-tetraedrische" Struktur angegeben worden ist (Johnson et al., Protein Sci. 1, (1992), 370-377; Matsumoto et al., J. Biol. Chem. 270 (1995), 19524-19531; G.H. Caughey, Am. J. Respir. Cell Mol. Biol. 16 (1997), 621-628).

Alle Tryptaseeinheiten des Tetramers sind nahezu identisch in ihrer Struktur und unterscheiden sich lediglich durch ihre relative Orientierung und durch die Kontakte zu ihren Nachbarn. Das Tetramer besitzt deshalb eine quasi- $2_2$ -Symmetrie, wobei die vier (quasi) äquivalenten Einheiten in einem rechteckigen, flachen Ring angeordnet sind. Von den vier Monomeren, die im folgenden im Uhrzeigersinn mit A, B, C und D bezeichnet werden (vgl. Figur 1), sind A mit C und B mit D identisch. Das Tryptasemonomer A berührt seinen Nachbarn B und D über zwei unterschiedliche Kontaktflächen, von etwa  $500$  bzw.  $1100 \text{ \AA}^2$ . Die Tryptaseeinheiten A und D (ebenso wie B und C), die über 2-zählige Rotationsachsen ineinander überführbar sind, sind miteinander durch eine langgestreckte periphere Brücke verbunden, wobei neben hydrophoben auch polare Wechselwirkungen zur Bindung beitragen. An der peripheren Oberfläche des A-D (und des entsprechenden B-C) Homodimers werden positive Ladungen durch angrenzende negative Ladungen ausgeglichen, was in einem relativ schwachen elektrostatischen Potential resultiert.

Im Gegensatz dazu ist die 2-zählige Symmetrie zwischen den Monomeren A und B (ebenso wie zwischen den Monomeren C und D) lokal gestört, und die beiden Monomeren berühren sich über eine vergleichsweise kleine und damit relativ gering stabile, hydrophobe Kontaktfläche. Diese zentrale, zirkuläre Kontaktfläche besteht ausschließlich aus hydrophoben Wechselwirkungen. Unter physiologischen Bedingungen wird das A-B (wie auch das C-D) Homodimer durch Heparinketten zusammengehalten, die an den positiv geladenen peripheren Flächen ansetzen. Das A-B-Homodimer (sowie das äquivalente C-D-Homodimer) trägt nämlich an seiner peripheren Oberfläche eine Reihe von positiv geladenen Resten, die ein positives elektrostatisches Potential bilden.

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Jedes Tryptase-Monomer besteht aus 246 Aminosäuren (vgl. Figur 4) und hat je nach Glykosilierungsgrad ein Molekulargewicht von 31 bis 34 kDa. Die Kernstruktur eines jeden Monomers besteht, ähnlich der aller anderen Trypsin-ähnlichen Serinproteinasen, aus zwei 6-strängigen  $\beta$ -Fässern (vgl. Figur 3). Diese  $\beta$ -Fässer werden durch drei Trans-Domänensegmente zusammengehalten und enthalten an ihrer Oberfläche weiterhin zwei Helizes und eine Reihe von Peptidschleifen. Die katalytischen Reste Ser195, His57 und Asp102 (die Bezeichnung erfolgt nach der sogenannten Chymotrypsinogen-Numerierung, die aufgrund der topologischen Ähnlichkeit zum Rinder-Chymotrypsinogen A definiert wird, vgl. Figur 4) sind in der Kontaktlinie zwischen den beiden Fässern angeordnet, während die aktive Zentrums-Spalte senkrecht zu beiden verläuft.

Der Tryptasekern, bestehend aus etwa 165 Resten, ist topologisch den Kernbereichen der Referenz-Proteinasen Trypsin und Chymotrypsin ähnlich. Die zusätzlichen Reste der Tryptase (15 bzw. 22) haben jedoch deutliche Konformationsunterschiede, insbesondere unterschiedliche Schleifenstrukturen. So zeigen sich drastische Unterschiede hinsichtlich Länge und Geometrie in sechs oberflächlichen Peptidschleifen, die das aktive Zentrum umstehen (die 70 bis 80er-Schleife, die 147er-Schleife mit dem anhängenden 152er-Sporn, die 37er-Schleife, die 60er-Schleife, die 170er-Schleife und die 97er-Schleife). Die Monomeren A und B berühren sich dabei über die drei erstgenannten Schleifen, während die Monomeren A und D über die drei letztgenannten Schleifen miteinander in Kontakt stehen. Die 60er-Schleife, die fünf insertierte Reste enthält, läuft abrupt von der Spalte weg Richtung Norden (die angegebenen relativen Richtungen beziehen sich auf die in Figur 2 gezeigte Orientierung), wo sie am cisPro 60 A knickt, um sich langsam dem allgemeinen Hauptkettenverlauf anderer Serinproteinasen anzunähern. Position 69, die in allen anderen homologen Proteinasen strikt für ein Gly vorbehalten ist, weist in Tryptase einen Arg-Rest auf. Die nachfolgende 70 bis 80er-Schleife, welche sich in den Calcium-bindenden Serinproteinasen um ein stabilisierendes Calciumion windet (Bode et al., J. Mol. Biol. 98 (1975) 693-717), ist in Tryptase kompakter und um drei Aminosäuren kürzer. Sie dient vermutlich nicht zur Calcium-Bindung, trotz topologisch ähnlicher

Ligandengruppen (Glu70, Asp80, Carbonyl 72 und 75). Die 97er Schleife, die den Nordrand der Spalte bildet, umfasst die gleiche Anzahl an Resten, die jedoch eine unterschiedliche Anordnung aufweisen: Ala97 nimmt die normalerweise durch den Rest 99 besetzte Position ein. Außerdem weist sie eine unübliche, zum Asp102 führende helikale Windung auf. Die 147er-Schleife (a/s "Autolyseschleife" in Pankreas-Proteinasen bezeichnet), die die Südwand der aktiven Spalte zusammen mit Gln192 bildet, ist um einen Rest kürzer bis Leu151. Die folgende, zwei Insertionsreste umfassende unübliche Pro152-Pro152A-cisPro152B-Phe153-Pro154-Sequenz bildet einen hydrophoben 152-"Sporn". Die mit neun Resten größte Insertion tritt in der 173-Schleife auf, welche der unüblich langen 3-wendigen "Zwischenhelix" (Helix  $\alpha 1$ , vgl. Figur 4) folgt. Die zehn Reste von His173 bis Val173I bilden eine verlängerte offene 173er-Biegung, die um die Imidazolseitenkette von His173 angeordnet ist.

Das aktive Zentrum und seine Umgebung sind im Trypsasemonomer in ihrer Struktur sehr ähnlich wie im Trypsin. Die sogenannte S1-Spezifitätstasche (mit P1, P2 usw. bzw. P1', P2' usw. werden im Folgenden die Peptidpositionen N- bzw. C-terminal der zu spaltenden Peptidbindung eines gebundenen Peptidsubstrats und mit S1, S2 etc. bzw. S1', S2' etc. die entsprechenden Bindungsstellen am Enzym bezeichnet), die sich links (hinsichtlich der sogenannten Standard-Orientierung, definiert durch eine horizontal verlaufende, dem Betrachter zugewandete aktive Zentrum-Spalte, in der gebundene Peptidsubstrate von links nach rechts laufen würden; vgl. Figur 3) vom reaktiven Ser195 öffnet, ist praktisch identisch zu der im Trypsin hinsichtlich der Konformation der umgebenden Hauptketten mit ihrem "Eingangsrahmen" Val213-Ser214-Trp215-Gly216-Glu217-Gly219-Cys220 (wobei Glu217 eine Ausnahme darstellt), ihrer "inneren Wand" Gly226-Ile227 (anstelle von Val) -Tyr228, ihrem "Boden" Asp189-Ser190-Cys191-Gln192-Gly193-Asp194-Ser195 und der abschließenden Disulfidbrücke Cys191 bis Cys220, und eignet sich zur Aufnahme von P1-Lysin- oder Arginin-Seitenketten.

In diese Tasche ragt die Amidinophenylgruppe der Amidinophenylbrenztraubensäure (APPA) hinein, in der gleichen Weise wie im APPA-Trypsin (Walter und Bode et al., Hoppe-Seylers Z. Physiol. Chem. 364 (1983), 949-959) und im APPA-Thrombin (Chen et al., Arch. Biochem. Biophys. 322 (1995), 198-203), wobei die Amidinogruppe der Carboxylatgruppe des Asp189 (am Boden der Tasche) gegenübersteht und zusätzliche Wasserstoffbrücken mit der Carbonylgruppe des Gly219 und dem Oy des Ser190 ausbildet und die Phenylgruppe eingeschlossen ist von den Peptidebenen 215 bis 216 und 190 bis 192. Die APPA-Pyruvatgruppe ragt aus der Tasche heraus, wobei sich die Carbonylgruppe unter Ausbildung eines tetraedrischen Übergangszustands (halbketal) an das Ser195 Oy anlagert. Unter der S1-Tasche (Standard-Orientierung) ragen, etwas getrennt durch die Gln192-Seitenkette, die Asp143-Seitenkette und (leicht nach links versetzt) die Asp147-Seitenkette aus der Moleküloberfläche heraus. Die resultierende negative Ladung ist ein möglicher zweiter Ankerpunkt für die basischen syntheti-

schen Tryptaseinhibitoren wie etwa Bis-benzamidine (Stürzebecher et al., Biol. Chem. Hoppe-Seyler 373 (1992) 1025-1030; Caughey et al., J. Pharmacol. Exp. Ther. 264 (1993), 676-682; Stubbs et al., J. Biol. Chem. 272 (1997), 19931-19937).

- 5 Die S2-Bindungsregion, nach oben begrenzt durch die flache Seite der His57-Imidazolgruppe und die Ala97-Seitenkette sowie (weiter außen) durch das Pro60A, ist etwas größer als im Trypsin. Die S3/S4-Region, auf der Indol-Gruppe des Trp215 und der Glu217-Seitenkette ruhend, ist dagegen nach oben durch die Gln98-Seitenkette desselben Monomers und die Tyr95-Phenolgruppe des Nachbarmonomers (D) in seiner Größe stark eingeschränkt. Den  
10 linken Rand der S6-Region bilden die Seitenketten des Pro60A und des Asp60B des Nachbarmonomers (D). Die S1' und die S2'-Regionen sind sehr ähnlich wie im Trypsin. Die S3'-Region wird dagegen rechts durch das vorspringende Pro37A stärker eingeschränkt, und eine mit gestreckter Konformation gebundene Peptidkette würde kurz nach dem P5'-Rest an Reste des Nachbarmonomers (B) anstossen. Die Subregionen S2 bis S6 der Monomere A und D (sowie  
15 der Monomere B und C) liegen in einer großen gemeinsamen Höhlung, die durch einen zusammenhängenden "Himmel", gebildet aus den vorspringenden 95er- 170er- und 60-er Peptidschleifen beider Monomeren, überwölbt wird und in der sich die S1 bis S4-Bindungsregionen der Monomeren A und D gegenüberstehen. Diese Geometrie, d.h. die räumliche Nähe der aktiven Zentren der Untereinheiten A und D (sowie der Unterheiten B und  
20 C) im Tetramer ermöglicht die Entwicklung von bifunktionalen Inhibitoren mit zwei entsprechend räumlich getrennten funktionalen Inhibitorgruppen die an zwei verschiedene, insbesondere benachbarte aktive Stellen in unterschiedlichen Monomerunterheiten des Tetramers binden. Die Verbindungslinie zwischen den beiden etwa 23 Å voneinander entfernten Ser195 Oγ-Atomen (sowie zwischen den jeweiligen S1-, S2-, S3-, S4- oder S1'-Subregionen) verläuft durch  
25 den freien Raum der stark negativ geladenen Höhle. Entsprechend ausgestaltete bifunktionelle Inhibitoren können deshalb beide katalytische Zentren durch diesen freien Raum miteinander verbinden.

- Die Erkenntnisse der Röntgenstrukturanalyse sind sehr hilfreich für die Entwicklung von  
30 spezifischen, in ihrer Geometrie optimierten Tryptaseinhibitoren.

- Bei den erfindungsgemäßen Inhibitoren handelt es sich um bifunktionelle Inhibitoren, d.h. Inhibitoren mit zwei bindefähigen, funktionellen Gruppen. Diese Gruppen sind derart ausgestaltet, dass sie spezifisch an aktive Stellen der Tryptase binden können. Bevorzugt binden  
35 die beiden funktionellen Gruppen des Inhibitors an aktive Stellen in verschiedenen Monomer-Untereinheiten des Tryptase-Tetramers.

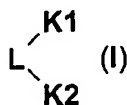
Die erfindungsgemäßen Inhibitoren sind zur Hemmung von humaner Tryptase geeignet. Unter

humaner Tryptase wird insbesondere das humane Enzym  $\beta$ -Tryptase mit der EC-Nr. 3.4.21.59 verstanden.

Die erfindungsgemäßen bifunktionellen Inhibitoren zeichnen sich dadurch aus, dass sie zwei  
 5 Kopfgruppen, hierin K1 und K2 genannt, umfassen, die durch einen Linker L verbunden sind. Die Kopfgruppen K1 und K2 können gleich oder verschieden sein und umfassen jeweils eine Gruppe Q, die mit einer Carboxylatgruppe Wechselwirkungen eingehen kann. Erfindungswesentlich ist, dass der Linker L eine Konformation einnehmen kann, sodass die Gruppen Q der beiden Kopfgruppen in einem Abstand von 20 bis 45 Å vorliegen. Dieses räumliche Erfordernis  
 10 ergibt sich aus der Raumstruktur der aktiven Zentren des Tryptasetetramers, wie sie durch Röntgenstruktur der Tryptase ermittelt wurde.

Weiterhin müssen die Ausmaße der Kopfgruppen und des Linkers der bifunktionellen Inhibitoren das Eindringen der Inhibitoren in einen Hohlraum mit den Dimensionen 52 Å x 32 Å x 40 Å  
 15 (Tiefe) erlauben. Die enge Öffnung des zentralen Kanals, die, wie oben ausgeführt, durch Peptidschleifen weiterhin verengt ist, verhindert das Eindringen von voluminösen Inhibitoren. Aus diesem Grund sind für andere Serin-Proteinasen bekannte proteinartige Inhibitoren bei Tryptase nicht wirksam. Eine wesentliche Anforderung an wirksame Inhibitoren von Tryptase ist deshalb eine räumliche Struktur, die ein Eindringen der Inhibitoren in den von den vier Tryptase-  
 20 Untereinheiten umschlossenen zentralen Hohlraum erlaubt. Es wurde überraschenderweise festgestellt, dass für die Struktur des Inhibitors nicht nur die unmittelbare Umgebung der Spezifitätstasche, sondern auch die räumliche Begrenzung hinsichtlich der durch die 4 Untereinheiten gebildeten und durch Peptidschleifen weiter verengten Pore von Bedeutung ist.

25 Die erfindungsgemäßen Inhibitoren weisen die Formel I



auf.

Die Kopfgruppen K1 und K2 der erfindungsgemäßen Inhibitoren umfassen bevorzugt Gruppen Q, die mit den Carboxylatgruppen von Asp189 von Tryptase Wechselwirkungen eingehen  
 30 können. Asp189 steht für die Aminosäure Asparaginsäure in Position 189 der einzelnen Aminosäuresequenzen der monomeren Untereinheiten der Tryptase bei Anwendung einer Zählweise in Analogie zu der für die Aminosäuresequenz des Chymotrypsins bekannten Zählweise (vgl. Figur 4). Der Abstand der Carboxylgruppen der Asp189-Reste wird an der Röntgenstruktur der Tryptase gemessen als die kürzeste Distanz zwischen den jeweiligen  
 35 Centroiden über die beiden endständigen Sauerstoffatome der Carboxylatgruppen. Die Abstände zwischen den Carboxylatgruppen der Asp189-Reste in den jeweiligen Untereinheiten

betragen zwischen A und B:  $45 \text{ \AA} \pm 1 \text{ \AA}$ , zwischen A und C  $45 \text{ \AA} \pm 1 \text{ \AA}$ , zwischen A und D  $33 \text{ \AA} \pm 1 \text{ \AA}$ , zwischen B und C  $33 \text{ \AA} \pm 1 \text{ \AA}$ , zwischen B und D  $45 \text{ \AA} \pm 1 \text{ \AA}$  und zwischen C und D  $45 \text{ \AA} \pm 1 \text{ \AA}$ .

- 5 Die Asp189-Reste sind Bestandteile der Spezifitätstaschen der aktiven Zentren der jeweiligen Untereinheiten. Ein erfindungsgemäß bevorzugter Tryptaseinhibitor umfasst somit zwei gleiche oder verschiedene Kopfgruppen K1 und K2, die jeweils eine Gruppe Q umfassen, die mit einer Carboxylatgruppe Wechselwirkungen eingehen kann, wobei die Kopfgruppen durch einen Linker L verbunden sind, wobei der Linker L in der Lage ist, eine Konformation einzunehmen, die den beiden Gruppen Q der Kopfgruppen K1 und K2 das Eingehen einer Wechselwirkung mit den Carboxylatgruppen der Asp189-Reste in den Spezifitätstaschen von zwei verschiedenen Untereinheiten der Tryptase ermöglicht, wobei der Linker so dimensioniert ist, dass er in den, von den vier Untereinheiten umschlossenen, zentralen Hohlraum passt. Bevorzugt kann der Linker L eine Konformation einnehmen, sodass die Gruppen Q der beiden Kopfgruppen in einem Abstand von 20 bis  $45 \text{ \AA}$  vorliegen, sodass eine Wechselwirkung mit den Carboxylatgruppen der Asp189-Reste der Untereinheiten A und D bzw. B und C möglich ist.

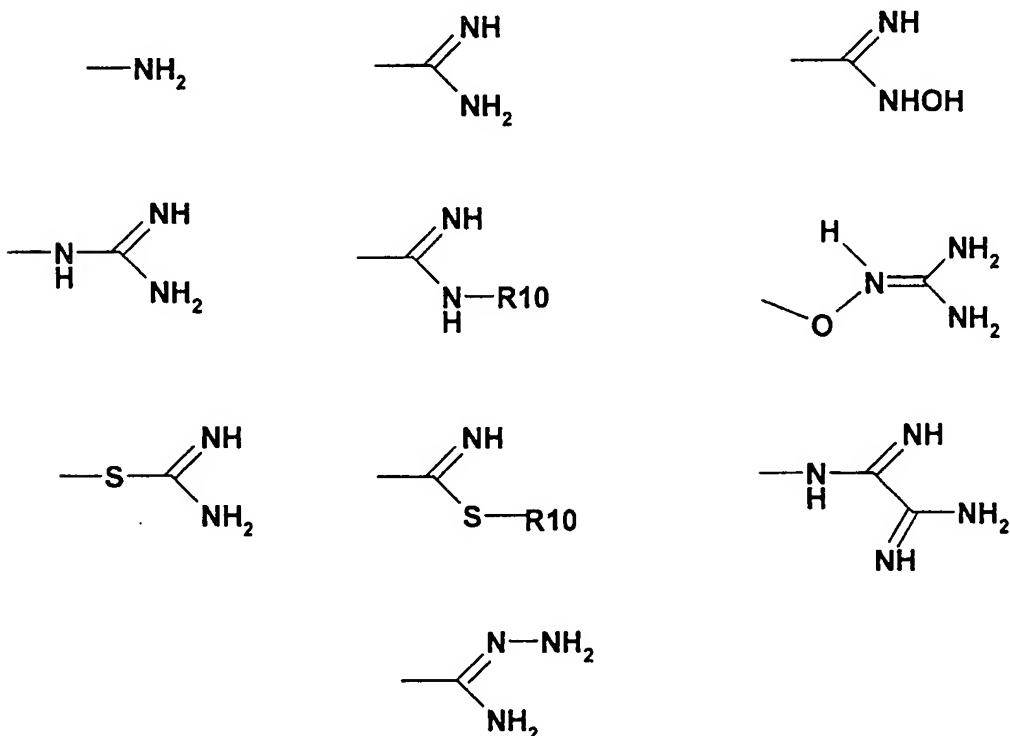
- Die Art der Wechselwirkung zwischen den Gruppen Q und den Carboxylatgruppen ist nicht beschränkt. Aufgrund der Bifunktionalität des Inhibitors wird auch bei geringen Wechselwirkungen eine hohe Bindungsaffinität und damit Spezifität des Inhibitors in Bezug auf Tryptase erzielt. Bevorzugt werden Gruppen Q verwendet, die mit Carboxylatgruppen, insbesondere mit den Carboxylatgruppen der Asp189-Reste in den Untereinheiten A und D bzw. B und C der Tryptase ionische Wechselwirkungen oder/und Wasserstoffbrücken-Wechselwirkungen eingehen können. Die Wechselwirkungen können dabei auch über ein oder mehrere Wassermoleküle vermittelt werden, wobei das Wassermolekül bzw. die Wassermoleküle zwischen der Kopfgruppe und der Carboxylatgruppe, insbesondere der Carboxylatgruppe des Asp189-Restes zu liegen kommen. Zur wirksamen Ausbildung der Wechselwirkungen, gegebenenfalls unter Einschluss eines oder mehrerer Wassermoleküle, weisen die Gruppen Q bevorzugt einen Abstand von etwa  $2,5$  bis  $5 \text{ \AA}$  von einem oder beiden Carboxylat-Sauerstoffatomen, insbesondere den Carboxylat-Sauerstoffatomen von Asp189 in der S1-Tasche auf.

- Der Linker L umfasst bevorzugt aromatische, heterocyclische, alicyclische oder aliphatische Gruppen. Die Gesamtgröße des Linkers bzw. des bifunktionellen Inhibitors ist grundsätzlich nicht begrenzt. Wesentlich für die Funktion als Tryptase-Inhibitor ist jedoch, dass die Ausmaße der Kopfgruppen und des damit verbundenen Linkerteils es ermöglichen, dass die funktionellen Gruppen Q mit den aktiven Stellen der Tryptase in Wechselwirkung treten. Dies ist dann gewährleistet, wenn die Ausmaße der Kopfgruppen und des Linkers das Eindringen der Inhibitoren in den durch die vier Trypsasemonomereinheiten im Tetramer gebildeten Hohlraum

bzw. Kanal ermöglichen. Hierbei ist insbesondere auch die Beschränkung des Eingangs des Kanals auf etwa 52 Å x 32 Å zu berücksichtigen. Ein erfindungsgemäß bevorzugter Inhibitor umfasst deshalb Kopfgruppen und einen Linker, die das Eindringen der Inhibitoren durch einen Eingang mit den Dimensionen 52 Å x 32 Å, bevorzugt 50 Å x 30 Å und besonders bevorzugt 40 Å x 25 Å erlauben. Ein solches Eindringen ist dann gewährleistet, wenn die Dimensionen der Kopfgruppen und des Linkers gleich oder kleiner als die oben angegebenen Dimensionen sind. Es ist aber auch möglich, einen Inhibitor zu verwenden, dessen Kopfgruppen und Linker an sich größer sind und die aufgrund von Konformationsänderungen des Inhibitors oder/und des Kanals der tetrameren Tryptase dennoch ein Eindringen erlauben.

10

Die erfindungsgemäßen bifunktionellen Inhibitoren zeichnen sich dadurch aus, dass sie gleichzeitig an zwei katalytische Zentren, insbesondere von zwei verschiedenen Tryptase-monomereinheiten binden können. Als Gruppe Q sind dabei alle Gruppen verwendbar, die mit einer Carboxylatgruppe Wechselwirkungen eingehen können. Bevorzugt stellt die Gruppe Q eine basische Gruppe, insbesondere einen Protonendonator dar. Besonders bevorzugt ist die Gruppe Q, ausgewählt aus

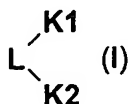


20 worin R10 1-4 C-Alkyl bedeutet. Erfindungsgemäß werden die funktionellen Gruppen Q, die Teil einer Kopfgruppe sein können oder eine Kopfgruppe selbst darstellen, durch geeignete Linker derart verbunden, dass die erfindungsgemäß beanspruchten Anforderungen an die Geometrie

erfüllt sind. Der Linker L kann dabei sowohl ein starres Strukturteil darstellen, sodass die Gruppen Q grundsätzlich im gewünschten Abstand von 20 bis 45 Å vorliegen. Er kann aber auch ein flexibles Strukturteil darstellen, solange es nur möglich ist, dass der Linker L eine Konformation einnehmen kann, in der die Gruppen Q in dem gewünschten Abstand von 20 bis 45 Å vorliegen.

Wie bereits erwähnt, ist die geometrische Anordnung der funktionellen Gruppen von grundsätzlicher Bedeutung für die Wirksamkeit ausgewählter Moleküle als bifunktionelle Inhibitoren von humaner Tryptase.

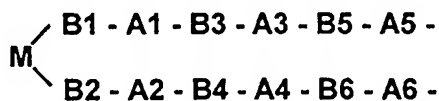
Ein erfindungsgemäß bevorzugter bifunktionseller Tryptase-Inhibitor weist daher die Formel I



auf,

wobei K1 und K2 gleich oder verschieden sind und jeweils eine Gruppe Q umfassen, die mit einer Carboxylatgruppe Wechselwirkungen eingehen kann,

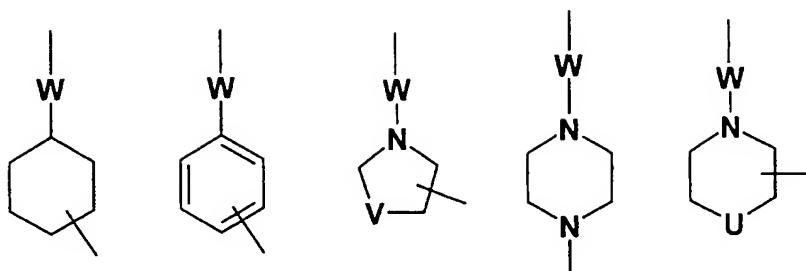
wobei der Linker L eine Konformation einnehmen kann, so daß die Gruppen Q der beiden Kopfgruppen in einem Abstand von 20 bis 45 Å vorliegen, wobei die Ausmaße der Kopfgruppen und des Linkers das Eindringen des Inhibitors in einen Hohlraum mit den Dimensionen 52 Å x 32 Å x 40 Å erlauben, und wobei L für



steht, worin

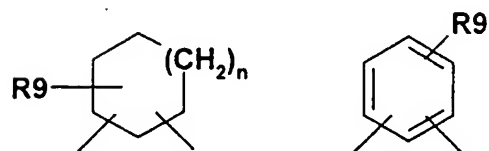
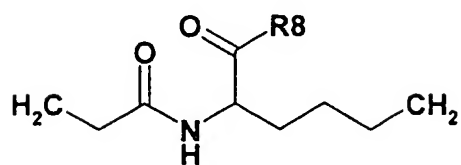
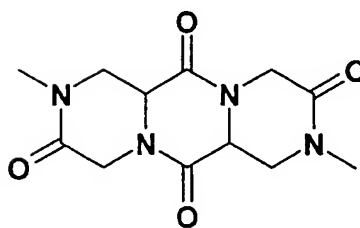
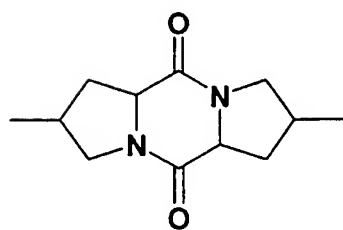
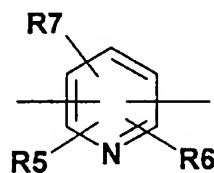
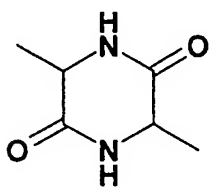
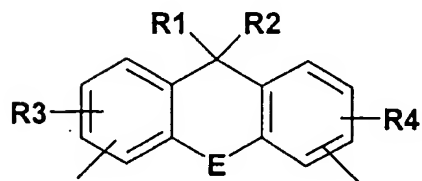
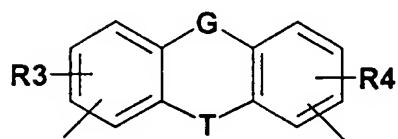
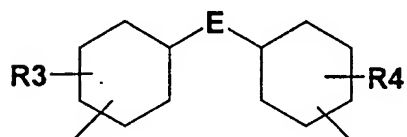
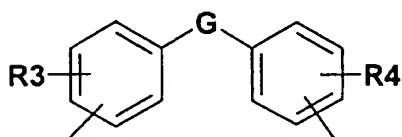
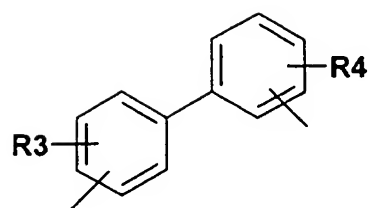
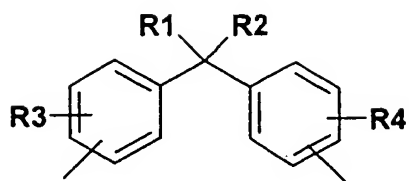
A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



wobei

- U     -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),  
 V     -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen) bedeutet, und  
 W     die Gruppe -C(O)- oder eine Bindung bedeutet,
- 5     A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,
- M     ausgewählt ist aus einer der nachfolgenden Gruppen



wobei

R1 und R2 gleich oder verschieden sind und Wasserstoff, 1-4C-Alkyl, ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl oder Hydroxy bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind  
5 -C(O)- bedeuten oder einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,

R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,

E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,

10 G -S-, -O- oder -S(O)<sub>2</sub>- bedeutet,

T -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,

R5 und R6 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,

R7 Wasserstoff, 1-4C-Alkyl, Phenyl oder Pyridyl bedeutet,

R8 1-4C-Alkoxy, N(R81)R82, Piperidino oder Morpholino bedeutet,

15 R81 und R82 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,

R9 Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeutet,

n 0, 1, 2 oder 3 bedeutet,

K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

20 K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

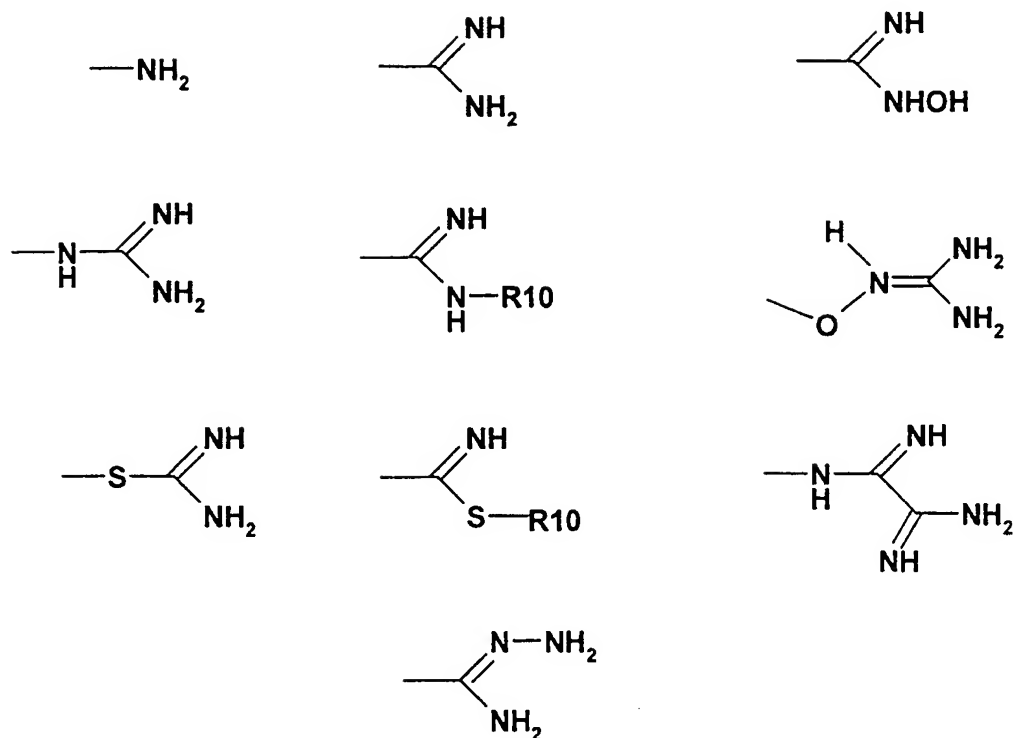
B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

25 m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und für einen 4-11C-Heteroaryl- oder 2-7C-Heterocycloalkylrest, enthaltend mindestens einen Ringstickstoff, der als Protonenakzeptor oder Protonendonator fungieren kann, stehen,

Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxy-carbonyl, 1-4C-Alkyl-carbonyloxy, Carboxyl oder Aminocarbonyl substituiert sein kann,

die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze,

wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

1-4C-Alkyl steht für geradkettige oder verzweigte Alkylreste mit 1 bis 4 Kohlenstoffatomen. Beispielsweise seien genannt der Butyl-, iso-Butyl-, sec.-Butyl-, tert.-Butyl-, Propyl-, Isopropyl-, Ethyl- und der Methylrest.

- 5 Als ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl seien beispielsweise der 2,2,3,3,3-Pentafluorpropyl-, der Perfluorethyl-, der 1,2,2-Trifluorethyl-, der 1,1,2,2-Tetrafluorethyl-, der 2,2,2-Trifluorethyl-, der Trifluormethyl- und der Difluormethylrest genannt.
- 10 Als 5- oder 6-gliedriger cyclischer Kohlenwasserstoff sei Cyclopentan oder Cyclohexan genannt.

1-4C-Alkoxy steht für Reste, die neben dem Sauerstoffatom einen geradkettigen oder verzweigten Alkylrest mit 1 bis 4 Kohlenstoffatomen enthalten. Beispielsweise seien genannt der

- 15 Butoxy-, iso-Butoxy-, sec.-Butoxy-, tert.-Butoxy-, Propoxy-, Isopropoxy- und bevorzugt der Ethoxy- und Methoxyrest.

1-4C-Alkylen steht für geradkettige oder verzweigte 1-4C-Alkylenreste, beispielsweise den Methylen-  $[-CH_2-]$ , Ethylen-  $[-CH_2-CH_2-]$ , Trimethylen-  $[-CH_2-CH_2-CH_2-]$ , Tetramethylen-  $[-CH_2-CH_2-CH_2-CH_2-]$ , 1,2-Dimethylethylen-  $[-CH(CH_3)-CH(CH_3)-]$ , 1,1-Dimethylethylen-  $[-C(CH_3)_2-CH_2-]$ , 2,2-Dimethylethylen-  $[-CH_2-C(CH_3)_2-]$ , Isopropyliden-  $[-C(CH_3)_2-]$  oder den 1-Methylethylenrest  $[-CH(CH_3)-CH_2-]$ .

- 25 1-3C-Alkylen steht für geradkettige oder verzweigte 1-3C-Alkylenreste, beispielsweise den Methylen-  $[-CH_2-]$ , Ethylen-  $[-CH_2-CH_2-]$ , Trimethylen-  $[-CH_2-CH_2-CH_2-]$ , Isopropyliden-  $[-C(CH_3)_2-]$  oder den 1-Methylethylenrest  $[-CH(CH_3)-CH_2-]$ .

Hat m die Bedeutung 0, so steht die Gruppe  $-(C(O))_m-$  für eine Bindung.

- 30 Hat p die Bedeutung 0, so steht die Gruppe  $-(C(O))_p-$  für eine Bindung.

Hat n die Bedeutung 0, so steht die Gruppe  $-(CH_2)_n-$  für eine Bindung.

- 35 4-11C-Heteroaryl steht für einen – gewünschtenfalls substituierten – mono- oder bicyclischen aromatischen Kohlenwasserstoff, der 4 bis 11 C-Atome und mindestens ein Ringstickstoffatom enthält; zusätzlich können ein oder mehrere der Kohlenstoffatome durch Ringheteroatome ausgewählt aus der Gruppe O, N oder S ersetzt sein. Im Falle von Bicyclen ist minde-

stens einer der Ringe aromatisch. Beispielhaft genannt seien Pyrid-4-yl, Pyrid-3-yl, Pyrimidin-5-yl, Imidazol-1-yl und Benzimidazol-5-yl.

2-7C-Heterocycloalkyl steht für einen – gewünschtenfalls substituierten – monocyclischen gesättigten oder teilweise gesättigten Kohlenwasserstoff, der 2 bis 7 C-Atome und mindestens ein Ringstickstoffatom enthält; zusätzlich können ein oder mehrere Kohlenstoffatome durch Ringheteroatome ausgewählt aus der Gruppe O, N oder S ersetzt sein. Beispielhaft genannt seien Piperid-4-yl, Piperazin-1-yl, Pyrrolidin-2-yl, Pyrrolidin-3-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl und Morpholin-2-yl.

10

5-12C-Arylen steht für einen – gewünschtenfalls substituierten – divalenten mono- oder bicyclischen aromatischen Kohlenwasserstoffrest, der 5 bis 12 C-Atome aufweist, wobei bei den bicyclischen aromatischen Kohlenwasserstoffresten mindestens einer der Ringe aromatisch ist. Die freien Valenzen können sich beide am aromatischen, beide am nichtaromatischen oder eine am aromatischen und eine am nichtaromatischen Ring befinden. Beispielhaft genannt seien 1,4-Phenylene, 1,3-Phenylene, 1,4-Naphthylene und 2,6-Naphthylene.

5-12C-Heteroarylen steht für einen Arylenrest, wie zuvor definiert, bei dem 1 bis 4 C-Atome durch Heteroatome ausgewählt aus der Gruppe O, N und S ersetzt sind. Beispielhaft genannt seien 2,5-Furylen, 2,5-Pyrrolylen, 4,2-Pyridylen, 5,2-Pyridylen, 2,5-Indolylen, 2,6-Indolylen, 3,5-Indolylen, 3,6-Indolylen, 3,5-Indazolylen, 3,6-Indazolylen, 2,5-Benzofuranylen, 2,6-Chinolinylen und 4,2-Thiazolylen.

3-8C-Cycloalkylen steht für einen – gewünschtenfalls substituierten – divalenten monocyclischen gesättigten oder teilweise gesättigten Kohlenwasserstoffrest, der 3 bis 8 C-Atome aufweist. Beispielhaft genannt seien der 1,3-Cyclopentylene-, der 1,3-Cyclohexylene- und bevorzugt der 1,4-Cyclohexylene-.

3-8C-Heterocycloalkylen steht für einen Cycloalkylenrest, wie zuvor definiert, bei dem 1 bis 3 C-Atome durch Heteroatome ausgewählt aus der Gruppe O, N und S ersetzt sind. Beispielhaft genannt seien der 1,4-Piperidinylen-, 1,4-Piperazinylen-, 2,5-Pyrrolidinylen-, 4,2-Imidazolidinylen- und bevorzugt der 4,1-Piperidinylenrest.

1-4C-Alkoxy-carbonyl steht für eine Carbonylgruppe, an die einer der vorstehend genannten 1-4C-Alkoxyreste gebunden ist. Beispielsweise seien der Methoxycarbonyl- ( $\text{CH}_3\text{O}-\text{C}(\text{O})-$ ) und der Ethoxycarbonylrest ( $\text{CH}_3\text{CH}_2\text{O}-\text{C}(\text{O})-$ ) genannt.

1-4C-Alkyl-carbonyloxy steht für eine Carbonyloxygruppe, an die einer der vorstehend

genannten 1-4C-Alkylreste gebunden ist. Beispielsweise sei der Acetoxyrest ( $\text{CH}_3\text{C}(\text{O})-\text{O}-$ ) genannt.

5 Mehrere der unter M aufgeführten Gruppen besitzen an sich oder aufgrund ihrer Substitution ein oder mehrere Chiralitätszentren. Die Erfindung umfaßt daher sowohl alle reinen Enantiomeren und alle reinen Diastereomeren, als auch deren Gemische in jedem Mischungsverhältnis.

10 Die Gruppen Z1 bzw. Z2 befinden sich definitionsgemäß zwischen den Gruppen B9 und B11 (-B9-Z1-B11-) bzw. B10 und B12 (-B10-Z2-B12-). Entsprechend steht bei den beispielhaft genannten divalenten Gruppierungen (z. B. 2,6-Indolylen) die erste Zahl für die Verknüpfungsstelle mit der Gruppe B9 bzw. B10 und die zweite Zahl für die Verknüpfungsstelle mit der Gruppe B11 bzw. B12.

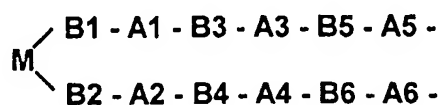
15 Als Salze kommen für Verbindungen der Formel I - je nach Substitution - alle Säureadditionssalze oder alle Salze mit Basen in Betracht. Besonders erwähnt seien die pharmakologisch verträglichen Salze der in der Galenik üblicherweise verwendeten anorganischen und organischen Säuren. Als solche eignen sich einerseits wasserlösliche und wasserunlösliche Säureadditionssalze mit Säuren wie beispielsweise Salzsäure, Bromwasserstoffsäure, Phosphorsäure, Salpetersäure, Schwefelsäure, Essigsäure, Zitronensäure, D-Gluconsäure, 20 Benzoessäure, 2-(4-Hydroxybenzoyl)-benzoessäure, Buttersäure, Sulfosalicylsäure, Maleinsäure, Laurinsäure, Äpfelsäure, Fumarsäure, Bernsteinsäure, Oxalsäure, Weinsäure, Embonsäure, Stearinsäure, Toluolsulfonsäure, Methansulfonsäure oder 3-Hydroxy-2-naphthoesäure, wobei die Säuren bei der Salzherstellung - je nachdem, ob es sich um eine ein- oder mehrbasige Säure handelt und je nachdem, welches Salz gewünscht wird - im äquimolaren oder einem davon abweichenden Mengenverhältnis eingesetzt werden.

30 Andererseits kommen auch Salze mit Basen in Betracht. Als Beispiele für Salze mit Basen seien Alkali- (Lithium-, Natrium-, Kalium-) oder Calcium-, Aluminium-, Magnesium-, Titan-, Ammonium-, Meglumin- oder Guanidiniumsalze erwähnt, wobei auch hier bei der Salzherstellung die Basen im äquimolaren oder einem davon abweichenden Mengenverhältnis eingesetzt werden.

35 Pharmakologisch unverträgliche Salze, die beispielsweise bei der Herstellung der erfindungsgemäßen Verbindungen im industriellen Maßstab als Verfahrensprodukte zunächst anfallen können, werden durch dem Fachmann bekannte Verfahren in pharmakologisch verträgliche Salze übergeführt.

- Dem Fachmann ist bekannt, daß die erfindungsgemäßen Verbindungen als auch ihre Salze, wenn sie zum Beispiel in kristalliner Form isoliert werden, verschiedene Mengen an Lösungsmitteln enthalten können. Die Erfindung umfaßt daher auch alle Solvate und insbesondere alle Hydrate der Verbindungen der Formel I, sowie alle Solvate und insbesondere alle Hydrate der Salze der Verbindungen der Formel I.

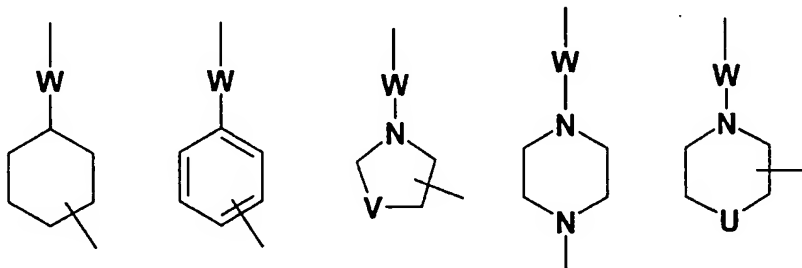
Eine Ausgestaltung (Ausgestaltung a) der erfindungsgemäßen Verbindungen der Formel I sind solche, worin L für



- 10 steht und

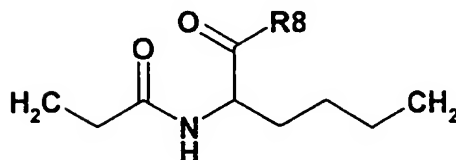
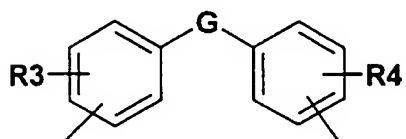
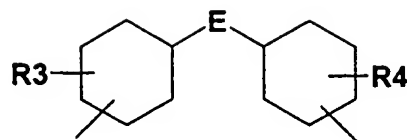
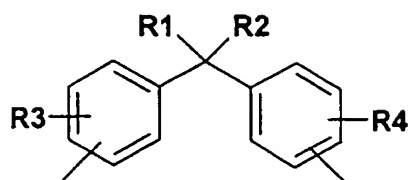
A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

- 15 A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



wobei

- U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),  
 V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und  
 20 W die Gruppe -C(O)- oder eine Bindung bedeutet,  
 A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,  
 M ausgewählt ist aus einer der nachfolgenden Gruppen



wobei

R1 und R2 gleich oder verschieden sind und Wasserstoff, 1-4C-Alkyl, ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl oder Hydroxy bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind  
5 -C(O)- bedeuten oder einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,

R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,

10 E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,

G -S-, -O- oder -S(O)<sub>2</sub>- bedeutet,

R8 1-4C-Alkoxy, N(81)R82, Piperidino oder Morpholino bedeutet,

R81 und R82 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,

K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

15 K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

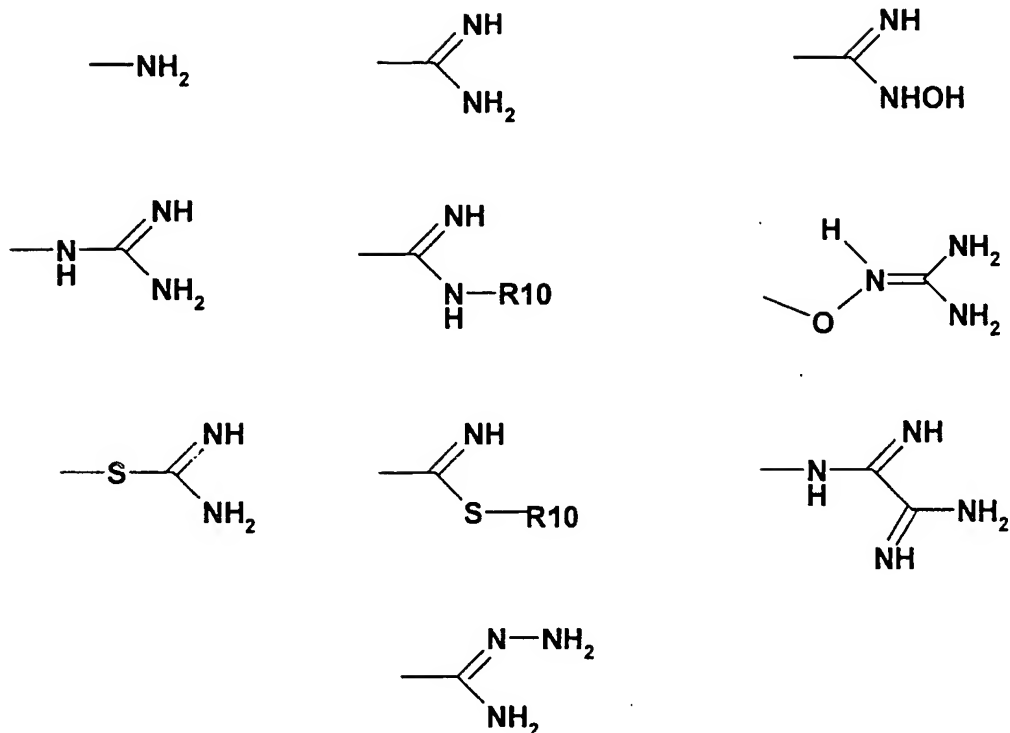
B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

20 m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und für einen 4-11C-Heteroaryl- oder 2-7C-Heterocycloalkylrest, enthaltend mindestens einen Ringstickstoff, der als Protonenakzeptor oder Protonendonator fungieren kann, stehen,

Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxycarbonyl, 1-4C-Alkylcarbonyloxy, Carboxyl oder Aminocarbonyl substituiert sein kann,

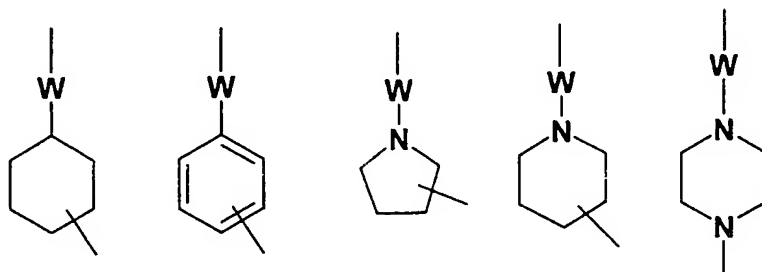
die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze,

wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

Hervorzuhebende Verbindungen der Ausgestaltung a sind solche, worin

A1 und A2 gleich oder verschieden sind und  $-C(O)-$ ,  $-NH-$ ,  $-O-$  (Sauerstoff),  $-C(O)-NH-$ ,  $-NH-C(O)-$ ,  $-O-C(O)-$ ,  $-C(O)-O-$  oder eine Bindung bedeuten,

- 5 A3 und A4 gleich oder verschieden sind und  $-C(O)-$ ,  $-O-$ ,  $-NH-$ ,  $-O-C(O)-$ ,  $-C(O)-O-$ ,  $-C(O)-NH-$ ,  $-NH-C(O)-$  oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe

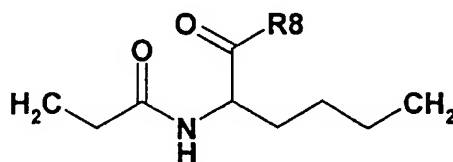
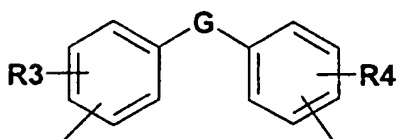
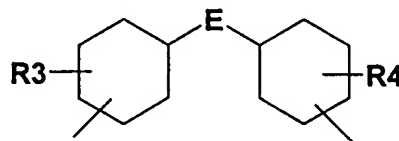
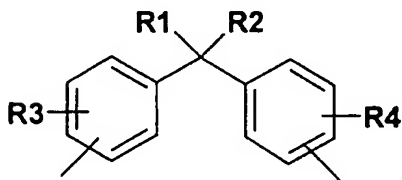


wobei

W die Gruppe  $-C(O)-$  oder eine Bindung bedeutet,

- 10 A5 und A6 gleich oder verschieden sind und  $-C(O)-$ ,  $-NH-$ ,  $-O-$ ,  $-C(O)-NH-$ ,  $-NH-C(O)-$ ,  $-O-C(O)-$ ,  $-C(O)-O-$  oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen



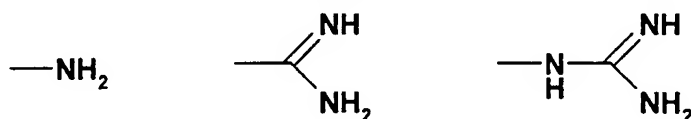
wobei

- 15 R1 und R2 gleich oder verschieden sind und Wasserstoff, 1-4C-Alkyl, ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl oder Hydroxy bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind  $-C(O)-$  bedeuten oder einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,

- 20 R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,

E  $-CH_2-$ ,  $-O-$  oder eine Bindung bedeutet,

- G -S-, -O- oder -S(O)<sub>2</sub>- bedeutet,
- R8 1-4C-Alkoxy, N(R81)R82, Piperidino oder Morpholino bedeutet,
- R81 und R82 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,
- K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,
- 5 K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,
- B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder geradkettiges oder verzweigtes 1-4C-Alkyl bedeuten,
- B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkyl bedeuten,
- 10 m 0 oder 1 bedeutet,
- p 0 oder 1 bedeutet,
- X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind

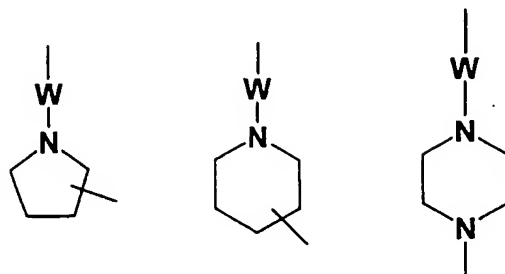


- Y1 und Y2 gleich oder verschieden sind und Piperid-4-yl, Piperid-3-yl, Piperazin-1-yl, Piperazin-2-yl, Morpholin-2-yl, Pyrrolidin-2-yl, Pyrrolidin-3-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, 2-Imidazolin-3-yl, 2-Imidazolin-2-yl, Imidazol-1-yl, Imidazol-2-yl, Imidazol-4-yl, 5-Methyl-Imidazol-4-yl, Pyrid-4-yl, Pyrid-3-yl, Pyridazin-4-yl, Pyrimidin-5-yl, Pyrimidin-4-yl, Indol-3-yl, Benzimidazol-4-yl oder Benzimidazol-5-yl bedeuten,
- 15
- Z1 und Z2 gleich oder verschieden sind und 1,4-Phenylen, 1,3-Phenylen, 1,4-Naphthylen, 2,6-Naphthylen, 1,4-Cyclohexylen, 1,3-Cyclohexylen, 1,3-Cyclopentylen, 1,4-Piperazinylen, 4,1-Piperidinylen, 1,4-Piperidinylen, 2,5-Pyrrolidinylen, 4,2-Imidazolidinylen, 2,5-Furylen, 2,5-Pyrrolylen, 4,2-Pyridylen, 5,2-Pyridylen, 6-Methyl-5,2-pyridinylen, 2,5-Indolylen, 2,6-Indolylen, 3,5-Indolylen, 3,6-Indolylen, 3,5-Indazolylen, 3,6-Indazolylen, 2,6-Chinolinylen, 2,5-Benzofuranylen oder 4,2-Thiazolylen bedeuten,
- 20
- die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer
- 25
- Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome oder Carbonylgruppen kommen würde.
- 30

Besonders hervorzuhebende Verbindungen der Ausgestaltung a sind solche, worin

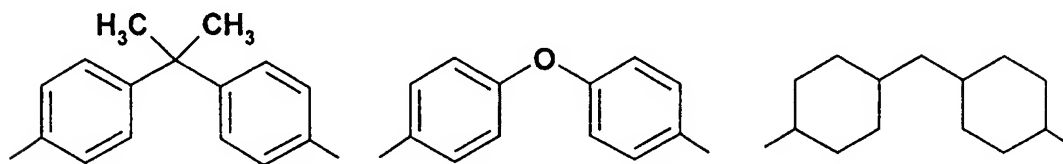
A1 und A2 gleich oder verschieden sind und -O- (Sauerstoff) oder -NH-C(O)- bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-NH- bedeuten oder ausgewählt sind aus der Gruppe



wobei W die Gruppe -C(O)- oder eine Bindung bedeutet,

- 5 A5 und A6 gleich oder verschieden sind und -C(O)-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten,  
 M ausgewählt ist aus einer der nachfolgenden Gruppen



- 10 K1 -B7-(C(O))<sub>m</sub>-B9-X1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,  
 K2 -B8-(C(O))<sub>p</sub>-B10-X2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,  
 B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder -CH<sub>2</sub>- (Methylen) bedeuten,  
 B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder  
 15 1-2C-Alkylen bedeuten,  
 m 0 oder 1 bedeutet,  
 p 0 oder 1 bedeutet,  
 X1 und X2 gleich oder verschieden sind und Amino, Amidino oder Guanidino bedeuten,  
 Z1 und Z2 gleich oder verschieden sind und 1,4-Phenylen, 1,3-Phenylen, 1,4-Cyclohexylen  
 20 oder 1,4-Piperazinylen bedeuten,

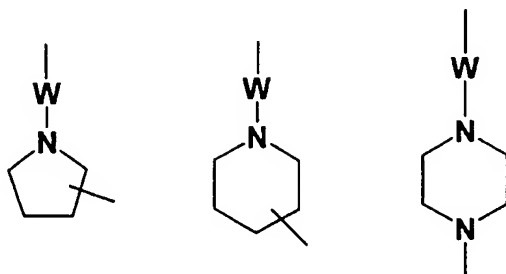
die Salze dieser Verbindungen, wobei alle diejenigen Verbindungen ausgeschlossen sind bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome oder zweier Carbonylgruppen kommen würde.

25

Bevorzugte Verbindungen der Ausgestaltung a sind solche, worin

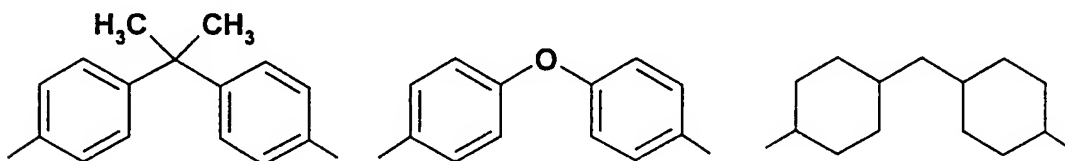
A1 und A2 gleich oder verschieden sind und -O- (Sauerstoff) oder -NH-C(O)- bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-NH- bedeuten oder ausgewählt sind aus der Gruppe



wobei W die Gruppe -C(O)- oder eine Bindung bedeutet,

- 5 A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-C(O)- oder eine Bindung bedeuten,  
M ausgewählt ist aus einer der nachfolgenden Gruppen

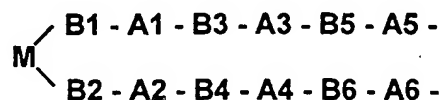


- K1 -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,  
10 K2 -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,  
B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder -CH<sub>2</sub>- (Methylen) bedeuten,  
B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder -CH<sub>2</sub>- (Methylen) bedeuten,  
15 m 0 oder 1 bedeutet,  
p 0 oder 1 bedeutet,  
X1 und X2 gleich oder verschieden sind und Amino, Amidino oder Guanidino bedeuten,  
Z1 und Z2 gleich oder verschieden sind und 1,4-Phenylen, 1,3-Phenylen, 1,4-Cyclohexylen oder 1,4-Piperazinylen bedeuten,  
20 die Salze dieser Verbindungen, wobei alle diejenigen Verbindungen ausgeschlossen sind bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome oder zweier Carbonylgruppen kommen würde.  
25 Besonders bevorzugte Verbindungen der Ausgestaltung a sind Bis{4-[4-(4-aminomethyl)cyclohexanoyl]piperazin-1-yl}carbonyl-4,4'-diamino-diphenylether, Bis{4-[(3-aminomethyl)-benzoyl]piperazin-1-yl}carbonyl-4,4'-diamino-diphenylether, Di{4-[4-(4-aminomethyl)cyclohexanoyl]-

amino]piperidin-1-yl-carbamoyl)cyclohexylmethan, 2,2-Bis-[4-(4-guanidiny]benzylamino)-  
carbonylmethoxyphenyl]propan, 2,2-Bis-[4-(10-amino-3,6-diaza-2,5-  
dioxodecyloxy)phenyl]propan und 2,2-Bis-[4-[4-(4-aminomethylbenzylcarbamoyl)-1-  
piperaziny]carbonyloxy]phenyl]propan, sowie die Salze dieser Verbindungen.

5

Eine weitere Ausgestaltung (Ausgestaltung b) der erfindungsgemäßen Verbindungen der  
Formel I sind solche, worin L für

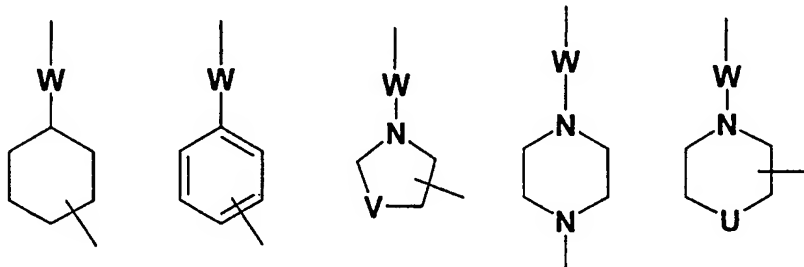


steht und

- 10 A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel),  
-S(O)<sub>2</sub>-, -S(O)<sub>2</sub>NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder ei-  
ne Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-,  
-C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind

- 15 aus der Gruppe



wobei

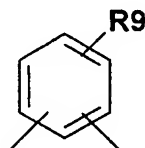
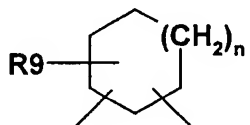
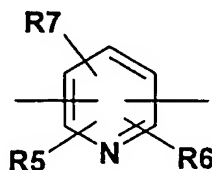
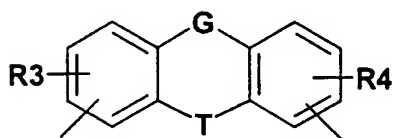
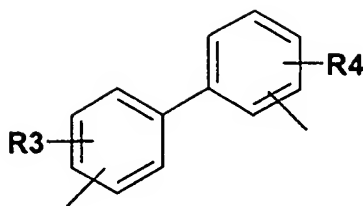
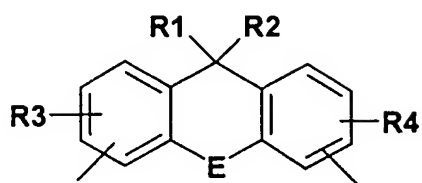
U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),

V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und

W die Gruppe -C(O)- oder eine Bindung bedeutet,

- 20 A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-,  
-O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen



wobei

R1 und R2 gleich oder verschieden sind und Wasserstoff, 1-4C-Alkyl, ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl oder Hydroxy bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind  
5 -C(O)- bedeuten oder einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,

R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,

10 E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,

G -S-, -O- oder -S(O)<sub>2</sub>- bedeutet,

T -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,

R5 und R6 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,

R7 Wasserstoff, 1-4C-Alkyl, Phenyl oder Pyridyl bedeutet,

15 R9 Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeutet,

n 0, 1, 2 oder 3 bedeutet,

K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

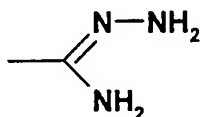
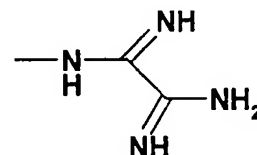
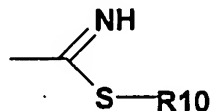
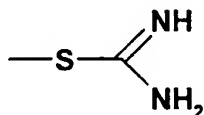
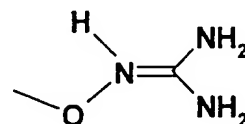
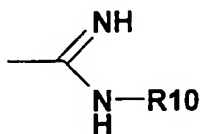
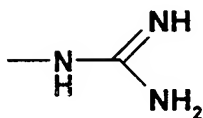
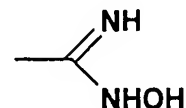
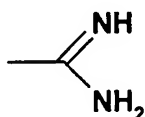
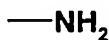
20 B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



5 wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und für einen 4-11C-Heteroaryl- oder 2-7C-Heterocycloalkylrest, enthaltend mindestens einen Ringstickstoff, der als Protonenakzeptor oder Protonendonator fungieren kann, stehen,

10 Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxy-carbonyl, 1-4C-Alkyl-carbonyloxy, Carboxyl oder Aminocar-

15 bonyl substituiert sein kann,  
die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der

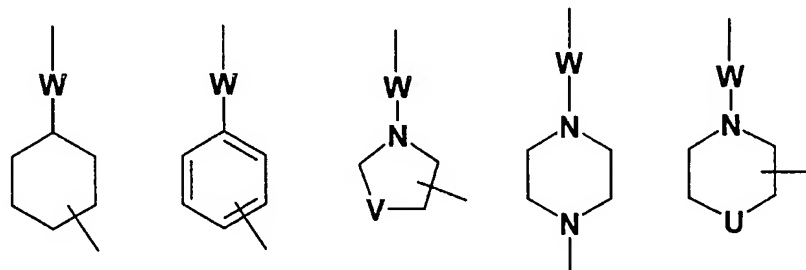
20 Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

Hervorzuhebende Verbindungen der Ausgestaltung b sind einerseits solche, worin

A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine

5 Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



wobei

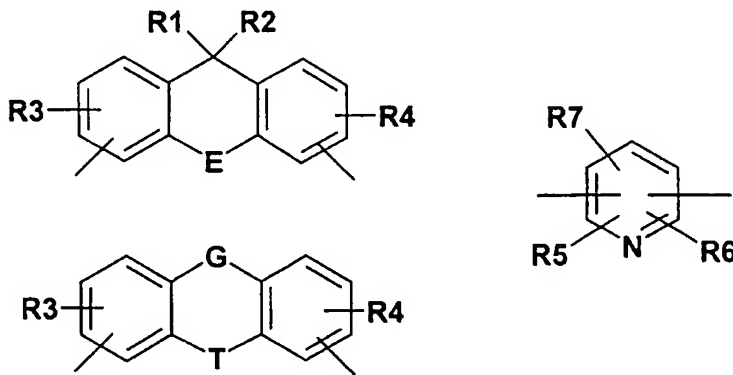
10 U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),

V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und

W die Gruppe -C(O)- oder eine Bindung bedeutet,

A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

15 M ausgewählt ist aus einer der nachfolgenden Gruppen



wobei

R1 und R2 gleich oder verschieden sind und ganz oder teilweise durch Fluor substituiertes

20 1-4C-Alkyl bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,

R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,

E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,

G -S(O)<sub>2</sub>- bedeutet,

5 T -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,

R5 und R6 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,

R7 Pyridyl bedeutet,

K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

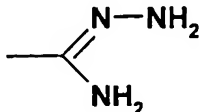
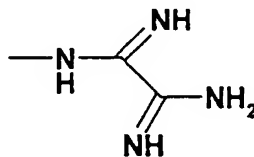
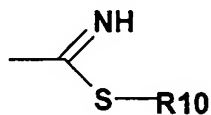
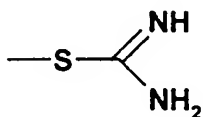
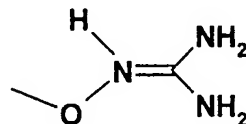
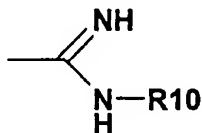
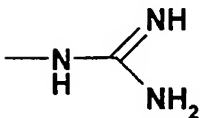
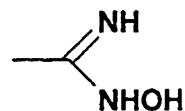
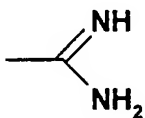
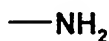
10 B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

m 0 oder 1 bedeutet,

15 p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und für einen 4-11C-Heteroaryl- oder 2-7C-Heterocycloalkylrest, enthaltend mindestens einen Ringstickstoff, der als Protonenakzeptor oder Protonendonator fungieren kann, stehen,

5 Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

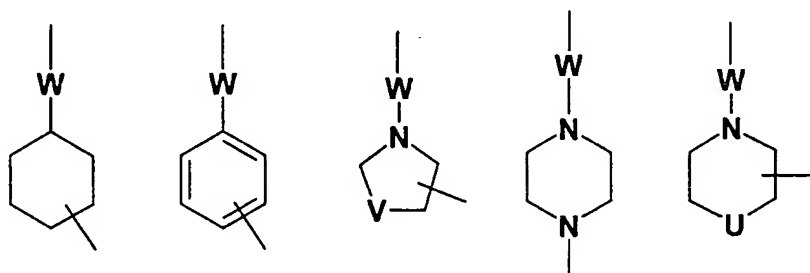
wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxycarbonyl, 1-4C-Alkylcarbonyloxy, Carboxyl oder Aminocarbonyl substituiert sein kann,

10 die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer  
15 Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

Hervorzuhebende Verbindungen der Ausgestaltung b sind andererseits solche, worin

20 A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



25 wobei

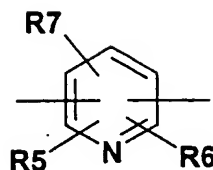
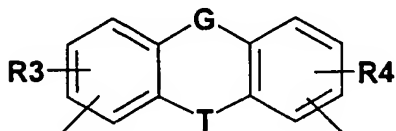
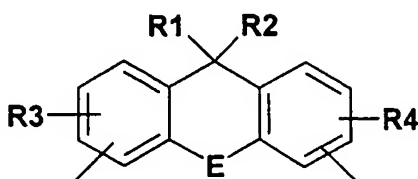
U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),

V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und

W die Gruppe -C(O)- oder eine Bindung bedeutet,

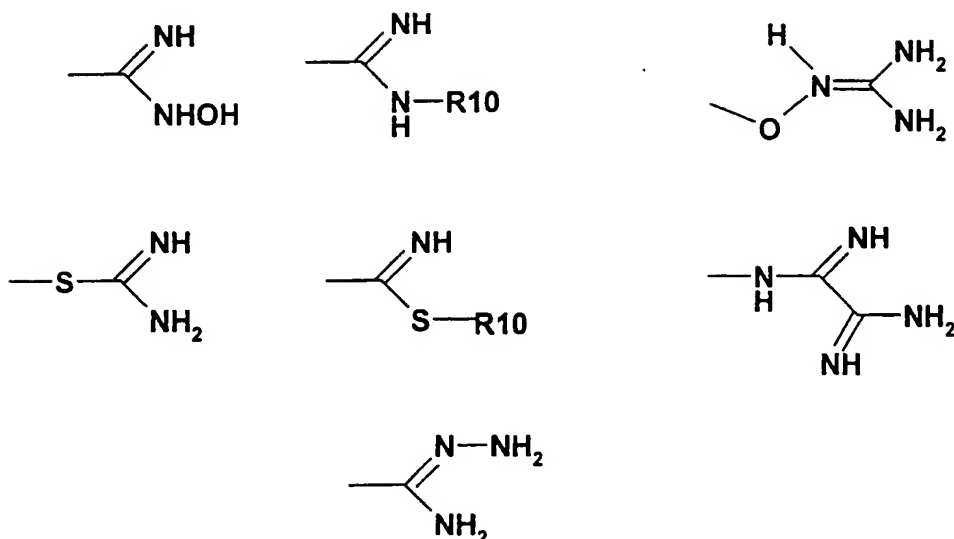
A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-,  
30 -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen



wobei

- 5 R1 und R2 gleich oder verschieden sind und 1-4C-Alkyl bedeuten oder gemeinsam und unter Einschluß des Kohlenstoffatoms, an das sie gebunden sind Carbonyl bedeuten,  
 R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,  
 E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,  
 10 G -O-(Sauerstoff) oder -S- (Schwefel) bedeutet,  
 T -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,  
 R5 und R6 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,  
 R7 Wasserstoff, 1-4C-Alkyl oder Phenyl bedeutet,  
 K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,  
 15 K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,  
 B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,  
 B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,  
 20 m 0 oder 1 bedeutet,  
 p 0 oder 1 bedeutet,  
 X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und Pyrrolidin-2-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, Pyridazin-4-yl, Indol-3-yl oder Morpholin-2-yl bedeuten,

- 5 Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

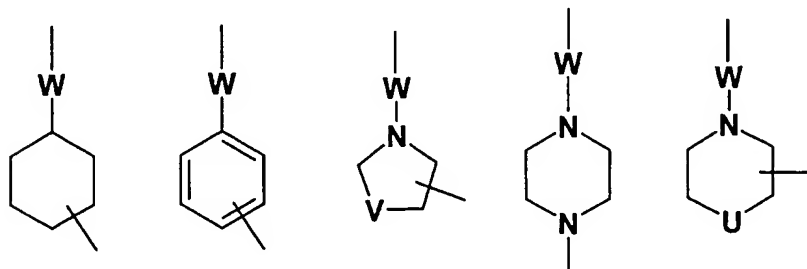
wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxycarbonyl, 1-4C-Alkylcarbonyloxy, Carboxyl oder Aminocarbonyl substituiert sein kann,

- 10 die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

- 20 Hervorzuhebende Verbindungen der Ausgestaltung b sind weiterhin solche, worin

A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -NH-S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



5 wobei

U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),

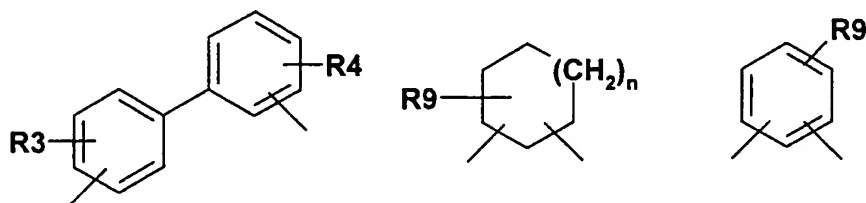
V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und

W die Gruppe -C(O)- oder eine Bindung bedeutet,

A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-,

10 -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen



wobei

15 R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,

R9 Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeutet,

n 0, 1, 2 oder 3 bedeutet,

20 K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

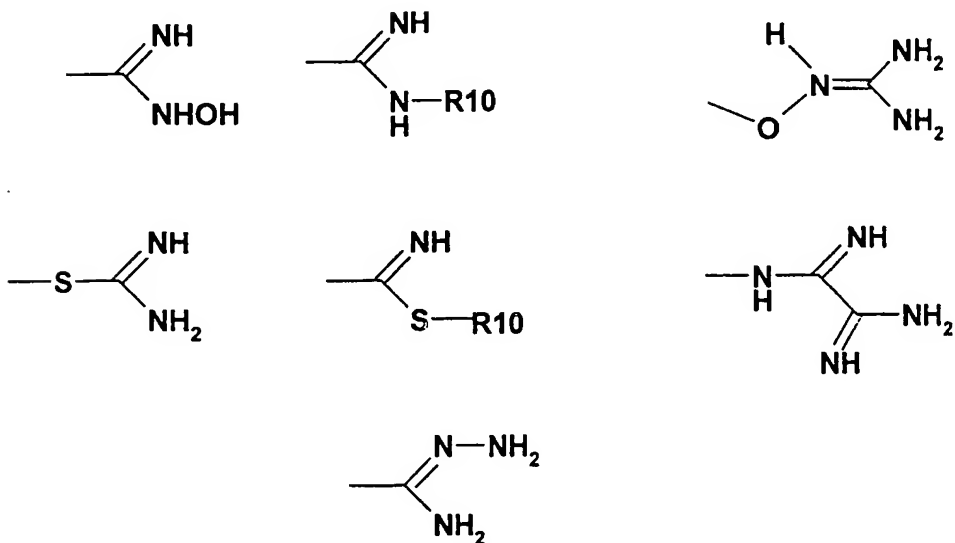
B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

25

m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

5 R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und Pyrrolidin-2-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, Pyridazin-4-yl, Indol-3-yl oder Morpholin-2-yl bedeuten,

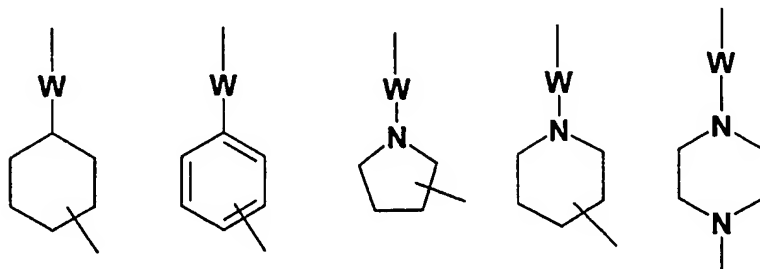
Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

10 wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxy-carbonyl, 1-4C-Alkyl-carbonyloxy, Carboxyl oder Aminocarbonyl substituiert sein kann,

15 die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier  
20 Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

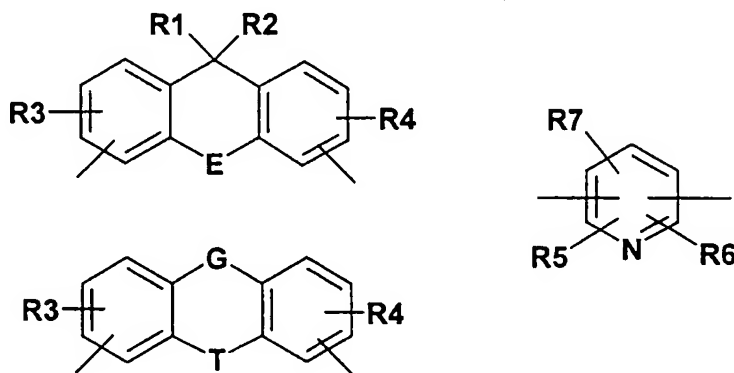
Besonders hervorzuhebende Verbindungen der Ausgestaltung b sind einerseits solche, worin A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -O-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



wobei

- 5 W die Gruppe -C(O)- oder eine Bindung bedeutet,  
 A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,  
 M ausgewählt ist aus einer der nachfolgenden Gruppen



10

wobei

- R1 und R2 gleich oder verschieden sind und ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,  
 15 R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,  
 E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,  
 G -S(O)<sub>2</sub>- bedeutet,  
 20 T -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,  
 R5 und R6 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,  
 R7 Pyridyl bedeutet,

K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,  
 K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,  
 B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen  
 bedeuten,

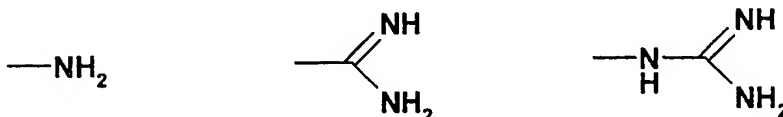
5 B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind

10



Y1 und Y2 gleich oder verschieden sind und Piperid-4-yl, Piperid-3-yl, Piperazin-1-yl, Piperazin-2-yl, Morpholin-2-yl, Pyrrolidin-2-yl, Pyrrolidin-3-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, 2-Imidazolin-3-yl, 2-Imidazolin-2-yl, Imidazol-1-yl, Imidazol-2-yl, Imidazol-4-yl, 5-Methyl-Imidazol-4-yl, Pyrid-4-yl, Pyrid-3-yl, Pyridazin-4-yl, Pyrimidin-5-yl, Pyrimidin-4-yl, Indol-3-yl, Benzimidazol-4-yl oder Benzimidazol-5-yl bedeuten,

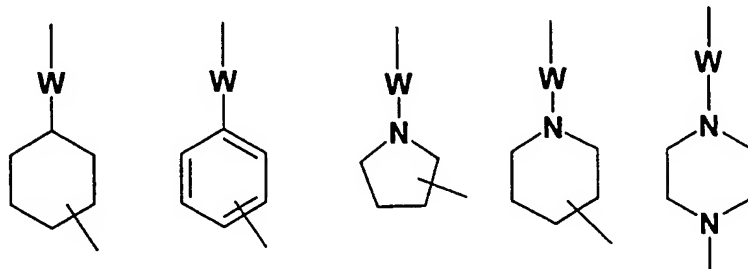
Z1 und Z2 gleich oder verschieden sind und 1,4-Phenylene, 1,3-Phenylene, 1,4-Naphthylene, 2,6-Naphthylene, 1,4-Cyclohexylene, 1,3-Cyclohexylene, 1,3-Cyclopentylene, 1,4-Piperazinylen, 4,1-Piperidinylen, 1,4-Piperidinylen, 2,5-Pyrrolidinylen, 4,2-Imidazolidinylen, 2,5-Furylen, 2,5-Pyrrolylen, 4,2-Pyridylen, 5,2-Pyridylen, 6-Methyl-5,2-pyridinylen, 2,5-Indolylen, 2,6-Indolylen, 3,5-Indolylen, 3,6-Indolylen, 3,5-Indazolylen, 3,6-Indazolylen, 2,6-Chinolinylen, 2,5-Benzofuranylen oder 4,2-Thiazolylen bedeuten,  
 die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden  
 25 Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze,  
 wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome oder zweier Carbonylgruppen kommen würde.

30

Besonders hervorzuhebende Verbindungen der Ausgestaltung b sind andererseits Verbindungen der Formel I worin

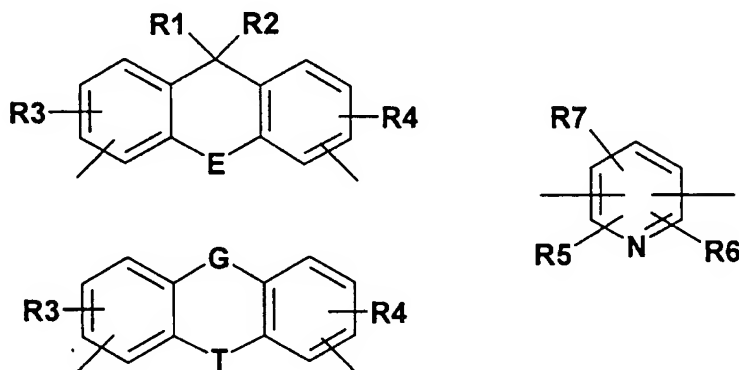
A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -O-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



wobei

- 5 W die Gruppe -C(O)- oder eine Bindung bedeutet,  
 A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,  
 M ausgewählt ist aus einer der nachfolgenden Gruppen



10

wobei

- R1 und R2 gleich oder verschieden sind und 1-4C-Alkyl bedeuten oder gemeinsam und unter Einschluß des Kohlenstoffatoms, an das sie gebunden sind Carbonyl bedeuten,  
 R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche  
 15 oder verschiedene 1-4C-Alkylreste bedeuten,  
 E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,  
 G -O- (Sauerstoff) oder -S- (Schwefel) bedeutet,  
 T -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,  
 R5 und R6 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,  
 20 R7 Wasserstoff, 1-4C-Alkyl oder Phenyl bedeutet,  
 K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,  
 K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

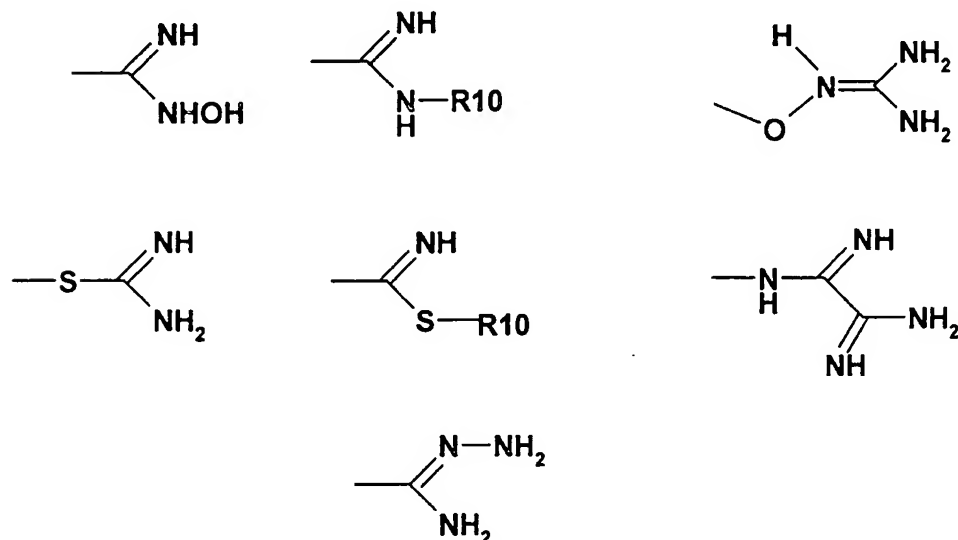
B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

5 m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

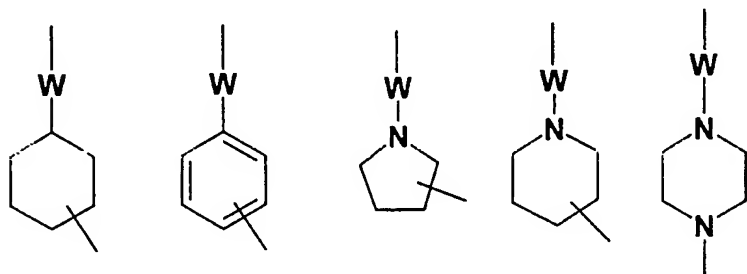
10 R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und Pyrrolidin-2-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, Pyridazin-4-yl, Indol-3-yl oder Morpholin-2-yl bedeuten,

Z1 und Z2 gleich oder verschieden sind und 1,4-Phenylen, 1,3-Phenylen, 1,4-Naphthylen, 2,6-Naphthylen, 1,4-Cyclohexylen, 1,3-Cyclohexylen, 1,3-Cyclopentylen, 1,4-Piperazinylen, 4,1-Piperidinylen, 1,4-Piperidinylen, 2,5-Pyrrolidinylen, 4,2-Imidazolidinylen, 2,5-Furylen, 2,5-Pyrrolylen, 4,2-Pyridylen, 5,2-Pyridylen, 6-Methyl-5,2-pyridinylen, 2,5-Indolylen, 2,6-Indolylen, 3,5-Indolylen, 3,6-Indolylen, 3,5-Indazolylen, 3,6-Indazolylen, 2,6-Chinolinylen, 2,5-Benzofuranylen oder 4,2-Thiazolylen bedeuten,

20 die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome oder  
25 zweier Carbonylgruppen kommen würde.

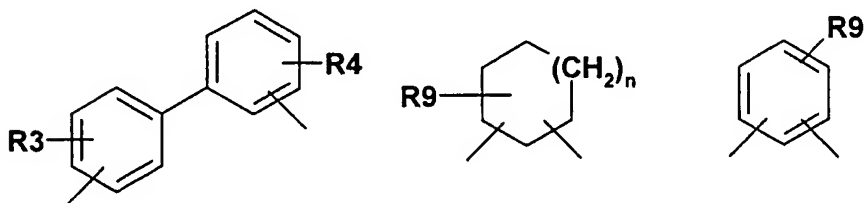
- Besonders hervorzuhebende Verbindungen der Ausgestaltung b sind weiterhin solche, worin A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,
- A3 und A4 gleich oder verschieden sind und -C(O)-, -O-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



wobei

W die Gruppe -C(O)- oder eine Bindung bedeutet,

- A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,
- M ausgewählt ist aus einer der nachfolgenden Gruppen

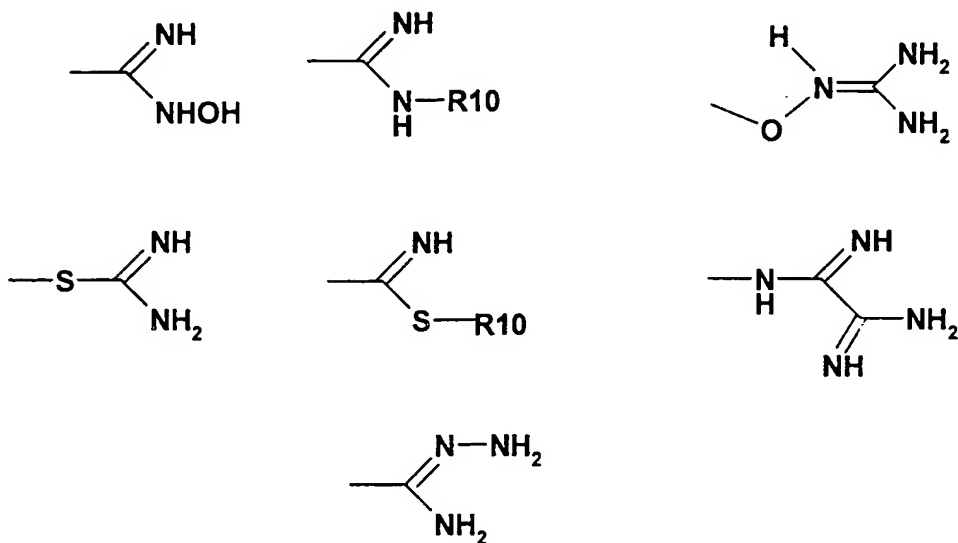


wobei

- R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,
- R9 Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeutet,
- n 0, 1, 2 oder 3 bedeutet,
- K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,
- K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,
- B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,
- B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,
- m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



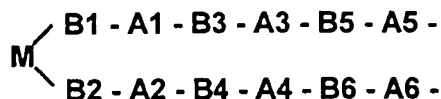
wobei

- 5 R10 1-4C-Alkyl bedeutet,  
 Y1 und Y2 gleich oder verschieden sind und Pyrrolidin-2-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, Pyridazin-4-yl, Indol-3-yl oder Morpholin-2-yl bedeuten,  
 Z1 und Z2 gleich oder verschieden sind und 1,4-Phenylene, 1,3-Phenylene, 1,4-Naphthylene, 2,6-Naphthylene, 1,4-Cyclohexylene, 1,3-Cyclohexylene, 1,3-Cyclopentylene, 1,4-Piperazine, 4,1-Piperidine, 1,4-Piperidine, 2,5-Pyrrolidine, 4,2-Imidazolidine, 2,5-Furylene, 2,5-Pyrrolylene, 4,2-Pyridylene, 5,2-Pyridylene, 6-Methyl-5,2-pyridinylen, 2,5-Indolylen, 2,6-Indolylen, 3,5-Indolylen, 3,6-Indolylen, 3,5-Indazolylen, 3,6-Indazolylen, 2,6-Chinolinylene, 2,5-Benzofuranylene oder 4,2-Thiazolylen bedeuten,  
 10 die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier  
 20 Carbonylgruppen kommen würde.

Besonders hervorzuhebende Verbindungen der Ausgestaltung b sind außerdem Pyridin-2,6-dicarbonsäure-bis-[4-(3-aminomethyl-benzoyl)-1-piperazid], Pyridin-2,6-dicarbonsäure-bis-[4-(trans-4-aminomethylcyclohexanoyl)-1-piperazid], 2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-[4-(3-aminomethyl-benzoyl)-1-piperazid], Pyridin-2,6-dicarbonsäure-bis-[4-(3-amino-

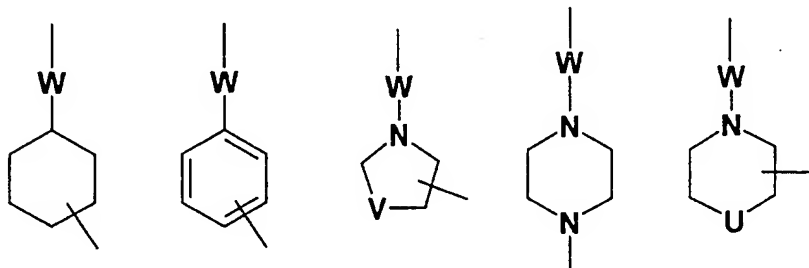
methyl-benzoylamino)-1-piperidid] und Pyridin-2,6-dicarbonsäure-bis-[4-(4-aminomethyl-cyclohexylcarbonylamino)-1-piperidid], sowie die Salze dieser Verbindungen.

- Eine weitere Ausgestaltung (Ausgestaltung c) der Verbindungen der Formel I sind solche,  
 5 worin L für



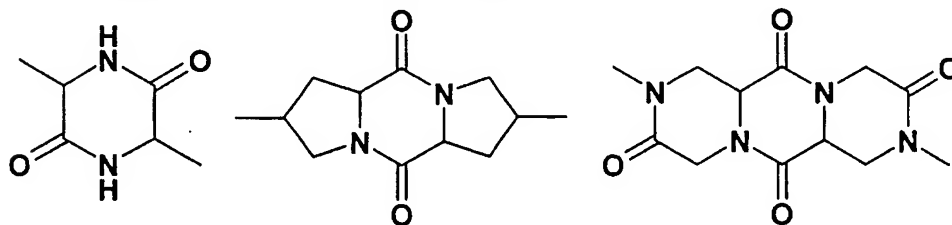
steht und

- A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel),  
 -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder ei-  
 10 ne Bindung bedeuten,  
 A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-,  
 -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind  
 aus der Gruppe



wobei

- 15 U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),  
 V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und  
 W die Gruppe -C(O)- oder eine Bindung bedeutet,  
 A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-,  
 -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,  
 20 M ausgewählt ist aus einer der nachfolgenden Gruppen



- K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

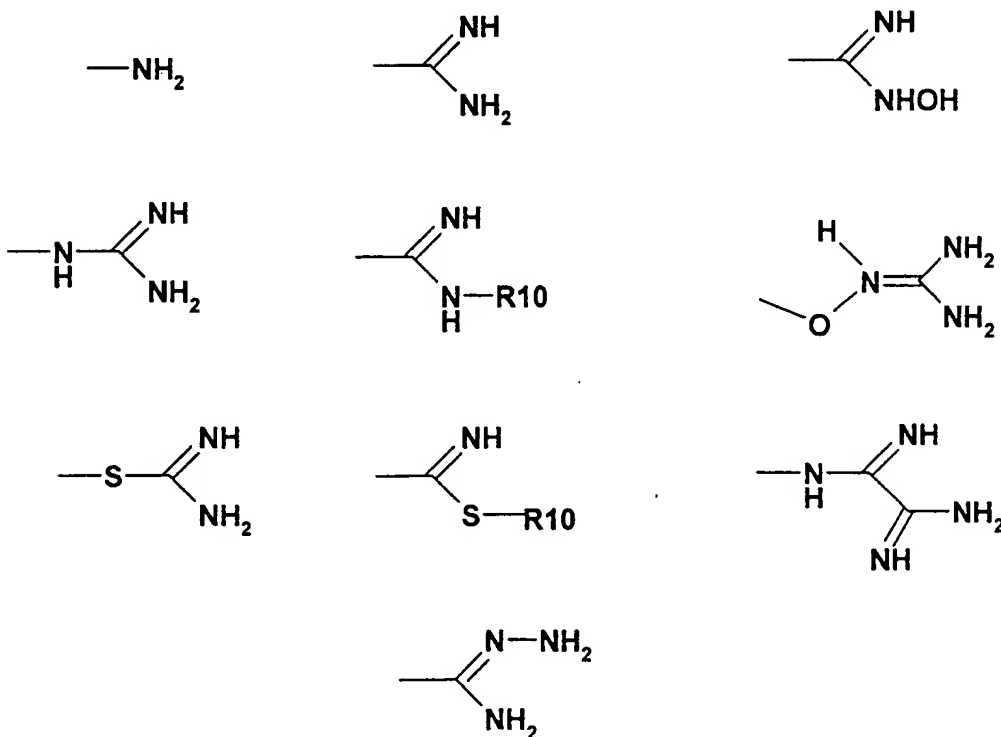
K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,  
B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen  
bedeuten,

B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Al-  
kylen bedeuten,

m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



10 wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und für einen 4-11C-Heteroaryl- oder 2-7C-Hetero-  
cycloalkylrest, enthaltend mindestens einen Ringstickstoff, der als Protonenakzeptor  
oder Protonendonator fungieren kann, stehen,

15 Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cy-  
cloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

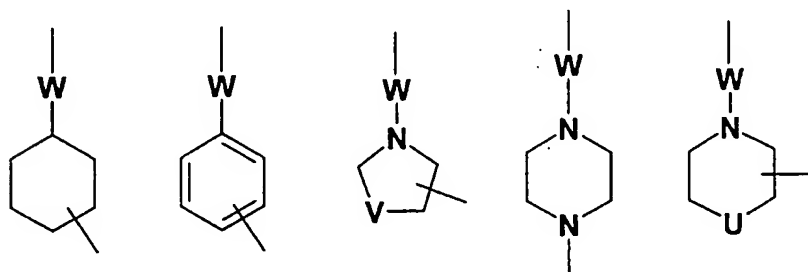
wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder  
Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten aus-  
gewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl,  
20 1-4C-Alkoxy, 1-4C-Alkoxycarbonyl, 1-4C-Alkylcarbonyloxy, Carboxyl oder Aminocar-  
bonyl substituiert sein kann,

- die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer
- 5 Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

Hervorzuhebende Verbindungen der Ausgestaltung c sind solche, worin

- A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel),
- 10 -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



- 15 wobei

U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),

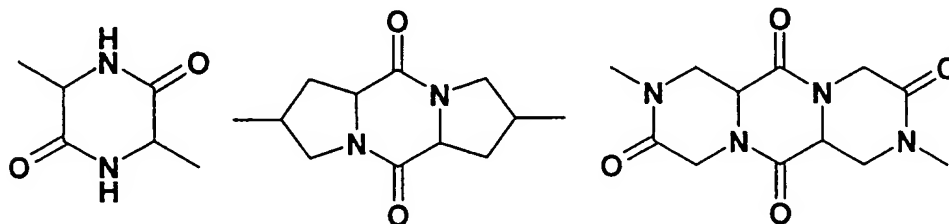
V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und

W die Gruppe -C(O)- oder eine Bindung bedeutet,

A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-,

- 20 -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen



K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

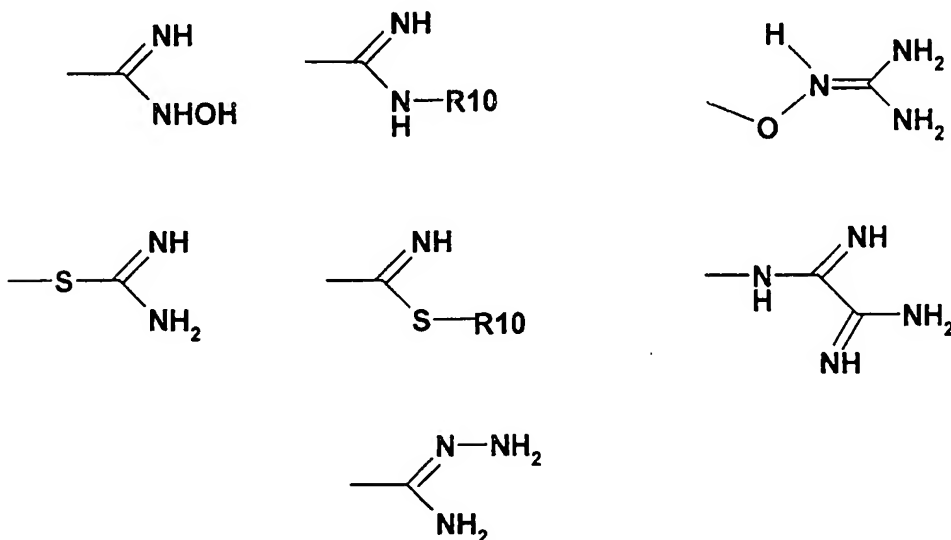
B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

5 m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

10 R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und Pyrrolidin-2-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, Pyridazin-4-yl, Indol-3-yl oder Morpholin-2-yl bedeuten,

Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

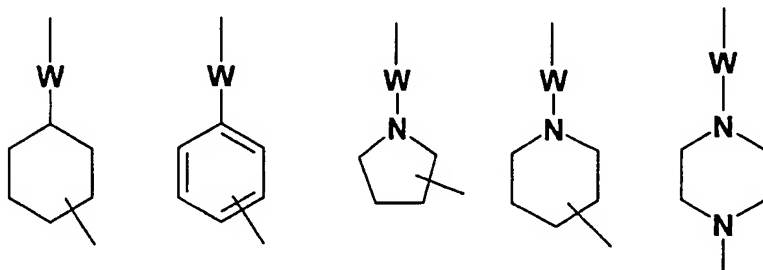
15 wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxycarbonyl, 1-4C-Alkylcarbonyloxy, Carboxyl oder Aminocarbonyl substituiert sein kann,

20 die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze, wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

Besonders hervorzuhebende Verbindungen der Ausgestaltung c sind solche, worin

A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

- 5 A3 und A4 gleich oder verschieden sind und -C(O)-, -O-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe

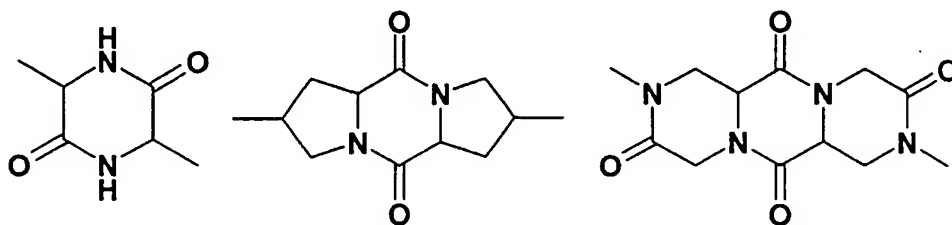


wobei

- 10 W die Gruppe -C(O)- oder eine Bindung bedeutet,

A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen



- 15 K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,

K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,

B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,

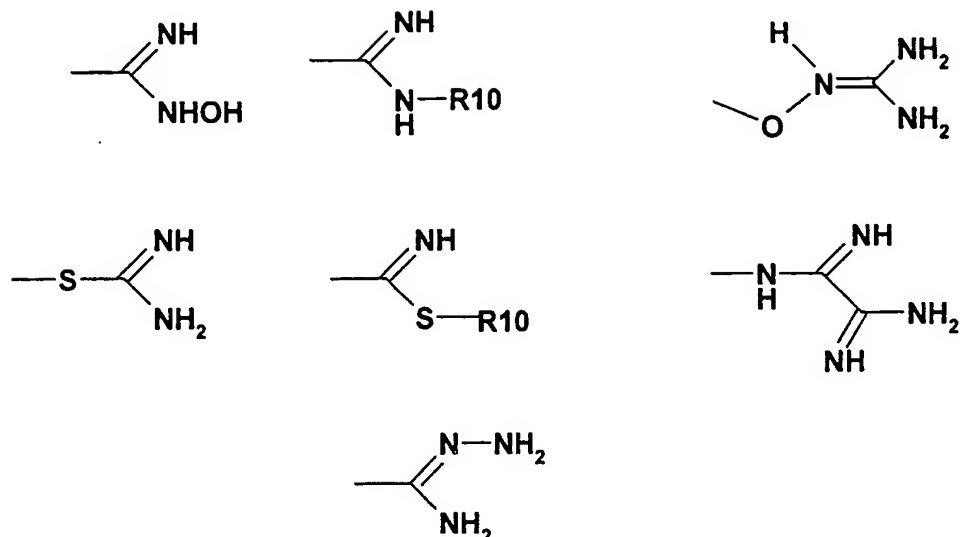
B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,

20

m 0 oder 1 bedeutet,

p 0 oder 1 bedeutet,

X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und Pyrrolidin-2-yl, Imidazolidin-1-yl, Imidazolidin-2-yl, Imidazolidin-4-yl, Pyridazin-4-yl, Indol-3-yl oder Morpholin-2-yl bedeuten,

- 5 Z1 und Z2 gleich oder verschieden sind und 1,4-Phenylen, 1,3-Phenylen, 1,4-Naphthylen, 2,6-Naphthylen, 1,4-Cyclohexylen, 1,3-Cyclohexylen, 1,3-Cyclopentylen, 1,4-Piperazinylen, 4,1-Piperidinylen, 1,4-Piperidinylen, 2,5-Pyrrolidinylen, 4,2-Imidazolidinylen, 2,5-Furylen, 2,5-Pyrrolylen, 4,2-Pyridylen, 5,2-Pyridylen, 6-Methyl-5,2-pyridinylen, 2,5-Indolylen, 2,6-Indolylen, 3,5-Indolylen, 3,6-Indolylen, 3,5-Indazolylen, 3,6-Indazol-

10 ylen, 2,6-Chinolinylen, 2,5-Benzofuranylen oder 4,2-Thiazolylen bedeuten,

die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze,

wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer

- 15 Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome oder zweier Carbonylgruppen kommen würde.

Neben der Wechselwirkung mit Asp189 können die Gruppen Q auch mit den funktionellen Gruppen einer oder mehrerer der Aminosäuren Carbonyl-Gly219, Carbonyl-Ser190 oder/und

- 20 Tyr228 der jeweiligen Tryptase-Untereinheit direkt oder unter Vermittlung von Wassermolekülen Wechselwirkungen eingehen.

Die Kopfgruppen K1 und/oder K2 können weitere funktionelle Gruppen aufweisen, die direkt oder unter Vermittlung von Wassermolekülen Wechselwirkungen zu funktionellen Gruppen

- 25 einer oder mehrerer der Aminosäuren Ser195 OY, Ser190 OY, Carbonyl-Ser190, Carbonyl-Gly216, Carbonyl-Gly219, NH-Gly219 und/oder Ser214 der jeweiligen Tryptase-Untereinheit

aufweisen. Die genauen Abstände zwischen den Bindungsstellen der Gruppen einer Tryptase-Untereinheit können den Kristallstrukturdaten entnommen werden.

5 Weiterhin können die Kopfgruppen K1 und/oder K2 bevorzugt eine geladene Gruppe umfassen, die Wasserstoff-Brückenwechselwirkungen mit Gln192 sowie elektrostatische Wechselwirkungen mit den Carboxylatgruppen von Asp143 oder/und Asp147 der Tryptase eingehen können.

Weiterhin kann der erfindungsgemäße bifunktionelle Inhibitor in den Kopfgruppen K1 und/oder K2 eine Gruppe aufweisen, die mit der S2-Region Wechselwirkungen eingehen kann.

10

Die Kopfgruppen K1 und/oder K2 können weiterhin eine Gruppe, bevorzugt eine kurze Gruppe, aufweisen, die eine Wechselwirkung mit den polaren oder unpolaren Seitenketten von Thr96, Ala97 und Gln98 und mit Tyr95 und Thr96 und Gln98 der benachbarten Untereinheiten (A und D bzw. B und C) der Tryptase in der S3/S4-Region eingehen kann.

15

Daneben können die Kopfgruppen K1 und/oder K2 auch positiv geladene Gruppen umfassen, die elektrostatische Wechselwirkungen mit der Carboxylatgruppe von Glu217 der Tryptase in der S3/S4-Tasche eingehen kann. Eine weitere Verbesserung der Gesamtbindung kann durch Kopfgruppen K1 und/oder K2 erzielt werden, die mit dem elektronegativen Feld um S3/S4 und S6 der Tryptaseeinheiten elektrostatische Wechselwirkungen eingehen können.

20

Die Erfindung umfaßt auch einen bifunktionellen Inhibitor wie oben beschrieben, bei dem die Gruppen Q der beiden Kopfgruppen durch den Linker L in einem Abstand von 34 bis 56 Å gehalten werden, sodass sie Wechselwirkungen mit den Carboxylatgruppen von Asp189 der Tryptaseuntereinheiten A und B oder A und C oder B und D oder C und D eingehen können.

25

Die Erfindung umfasst sowohl symmetrische als auch unsymmetrische bifunktionelle Inhibitoren. Wesentlich ist, dass die Kopfgruppen in einem Abstand vorliegen, der ihre Wechselwirkung mit der Substrat-Spezifitätstasche der einzelnen Tryptaseuntereinheiten ermöglicht.

30

Die erfindungsgemäßen Inhibitoren weisen bevorzugt einen  $K_i$ -Wert  $< 100 \mu\text{mol}$ , insbesondere  $< 1 \mu\text{mol}$ , besonders bevorzugt  $< 100 \text{ nmol}$  und am meisten bevorzugt  $< 10 \text{ nmol}$  auf.

Die Erfindung umfasst auch einen bifunktionellen Inhibitor wie oben beschrieben, der eine oder zwei weitere funktionelle Gruppen Q umfasst, die derart angeordnet sind, dass sie mit weiteren Substrat-Spezifitätstaschen von weiteren Tryptase-Monomeren des Tryptase-Tetramers Wechselwirkungen eingehen können. Ein solcher multifunktioneller Inhibitor muss geometrisch derart ausgestaltet sein, dass er für die funktionellen Gruppen Q sowie für die Gesamtgröße des

35

Moleküls die in Figur 1 angegebenen geometrischen Rahmenbedingungen erfüllt.

Die Verbindungen der Formel I setzen sich aus einer Vielzahl divalenter Bausteine (M, A1, A2, A3, A4, A5, A6, B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11, B12, Z1 und Z2) zusammen. Ihre Synthese kann grundsätzlich ausgehend von jedem dieser Bausteine erfolgen. Bei weitgehend symmetrisch aufgebauten Verbindungen der Formel I ist der Aufbau beginnend vom Zentralbaustein M bevorzugt, während bei überwiegend unsymmetrischen Verbindungen der Formel I die Synthese ausgehend von einem der Endgruppen K1 oder K2 vorteilhaft sein kann.

10

Die Verknüpfung der Bausteine erfolgt dabei immer nach dem gleichen, dem Fachmann an sich bekannten Muster.

Dem Fachmann ist bekannt, daß die Verbindungen der Formel I entweder Baustein für Baustein aufgebaut werden können, oder daß zunächst größere aus mehreren Einzelbausteinen bestehende Fragmente erstellt werden können, die anschließend zum Gesamtmolekül zusammengesetzt werden.

Aufgrund der Bedeutungen, die die einzelnen Bausteine der Verbindungen der Formel I annehmen können, treten in den Verbindungen der Formel I Amino- [-NH-], Ether [-O-], Thioether [-S-], Keto- [-C(O)-], Thioketo- [-C(S)-], Sulfonyl- [-S(O)<sub>2</sub>-], Ester- [-O-C(O)-, -C(O)-O-], Amid- [-C(O)-NH-, -NH-C(O)-], Sulfonamid [-SO<sub>2</sub>-NH-, -NH-SO<sub>2</sub>-], Carbamat [-NH-C(O)-O-, -O-C(O)-NH-], Carbamid- (-NH-C(O)-NH-) oder Carbonatbrücken [-O-C(O)-O-] auf.

25

Die Art und Weise, wie solche Brücken hergestellt werden, sind dem Fachmann an sich bekannt, geeignete Methoden und Ausgangsverbindungen zu ihrer Herstellung werden beispielsweise in March, Advanced Organic Chemistry, Reactions, Mechanisms and Structure, Third Edition, 1985, John Wiley & Sons beschrieben.

30

Ether- und Thioetherbrücken können beispielsweise nach der Methode von Williamson hergestellt werden.

Keto- oder Thioketobrücken können beispielsweise als Bestandteil größerer Bausteine, wie z. B. dem 1,3-Dichloraceton eingeführt werden.

35

Sulfonylbrücken können beispielsweise durch Oxidation von Thioetherbrücken erhalten werden.

Für den Aufbau von Esterbrücken ist eine Vielzahl von Methoden bekannt. Beispielhaft genannt sei hier die Umsetzung von Säuren mit Alkoholen, vorzugsweise unter Verwendung von  $H_2SO_4$  oder p-Toluolsulfonsäure als Katalysator; oder unter Zugabe eines wasserentziehenden Mittels, wie zum Beispiel Molekularsieb oder einem Carbodiimid. Desweiteren kann hier die Umsetzung von Säurechloriden mit Alkoholen genannt werden.

Auch für die Darstellung von Amidbrücken gibt es eine Vielzahl bekannter Methoden. Als Beispiel sei hier die Umsetzung von Säurechloriden mit primären oder sekundären Aminen genannt. Desweiteren sei auch auf all die Methoden verwiesen, die für die Peptidchemie entwickelt wurden. Entsprechend lassen sich aus Sulfonsäurechloriden und primären oder sekundären Aminen Sulfonamidbrücken aufbauen.

Carbamatbrücken können z. B. durch Reaktion von Chlorkohlensäureestern mit Aminen hergestellt werden. Die Chlorkohlensäureester ihrerseits können aus Alkoholen und Phosgen aufgebaut werden. Eine weitere Variante zum Aufbau von Carbamatbrücken stellt die Addition von Alkoholen an Isocyanate dar.

Ähnlich wie bei den Carbamatbrücken können ausgehend von Chlorkohlensäureestern durch Umsetzung mit Alkoholen (anstatt Aminen) Carbonatbrücken hergestellt werden.

Carbamidbrücken lassen sich z. B. durch die Reaktion von Isocyanaten mit Aminen herstellen.

Die N-Oxidation erfolgt auf eine dem Fachmann ebenfalls vertraute Weise, z.B. mit Hilfe von m-Chlorperoxybenzoesäure in Dichlormethan bei Raumtemperatur. Welche Reaktionsbedingungen für die Durchführung des Verfahrens im einzelnen erforderlich sind, ist dem Fachmann aufgrund seines Fachwissens geläufig.

Die Isolierung und Reinigung der erfindungsgemäßen Substanzen erfolgt in an sich bekannter Weise z.B. derart, daß man das Lösungsmittel im Vakuum abdestilliert und den erhaltenen Rückstand aus einem geeigneten Lösungsmittel umkristallisiert oder einer der üblichen Reinigungsmethoden, wie beispielsweise der Säulenchromatographie an geeignetem Trägermaterial, unterwirft.

Salze erhält man durch Auflösen der freien Verbindung in einem geeigneten Lösungsmittel, z.B. in einem chlorierten Kohlenwasserstoff, wie Methylenchlorid oder Chloroform, oder einem niedermolekularen aliphatischen Alkohol (Ethanol, Isopropanol), das die gewünschte

Säure bzw. Base enthält, oder dem die gewünschte Säure bzw. Base anschließend zugegeben wird. Die Salze werden durch Filtrieren, Umfällen, Ausfällen mit einem Nichtlösungsmittel für das Anlagerungssalz oder durch Verdampfen des Lösungsmittels gewonnen. Erhaltene Salze können durch Alkalisierung bzw. durch Ansäuern in die freien Verbindungen  
5 umgewandelt werden, welche wiederum in Salze übergeführt werden können. Auf diese Weise lassen sich pharmakologisch nicht verträgliche Salze in pharmakologisch verträgliche Salze umwandeln.

Die Herstellung von Verbindungen der Formel I sei exemplarisch an Hand der nachfolgenden  
10 Beispiele 4-14 und der Figuren 8-19 aufgezeigt. Weitere Verbindungen der Formel I können analog oder unter Anwendung der oben aufgeführten, dem Fachmann an sich bekannten Methoden hergestellt werden.

Die Erfindung betrifft weiterhin humane Tryptase in kristallisierter Form. Eine solche kristallisierte Tryptase war bisher im Stand der Technik nicht bekannt, ist aber hilfreich für die  
15 Entwicklung von Tryptaseinhibitoren. Eine solche kristallisierte humane Tryptase ist insbesondere durch die tetragonale Raumgruppe  $P4_1$  und die Zellachsen  $a = b = 83 \text{ \AA} \pm 5 \text{ \AA}$  und  $c = 127 \text{ \AA} \pm 5 \text{ \AA}$ , bevorzugt  $a = b = 83 \text{ \AA} \pm 2 \text{ \AA}$  und  $c = 127 \text{ \AA} \pm 2 \text{ \AA}$  und besonders bevorzugt  $a = b = 83 \text{ \AA} \pm 1 \text{ \AA}$  und  $c = 127 \text{ \AA} \pm 1 \text{ \AA}$  charakterisiert. Die Kristalle enthalten ein Tryptasetetramer pro  
20 asymmetrischer Einheit.

Die Erfindung betrifft weiterhin ein Verfahren zur Herstellung von humaner Tryptase in kristallisierter Form, welches dadurch gekennzeichnet ist, dass die Kristalle durch Dampfdiffusion oder Dialyse erhalten werden. Es ist auch möglich, ein anderes, dem Fachmann  
25 bekanntes, übliches Kristallisationsverfahren einzusetzen. Zur Kristallisierung wird das Protein bevorzugt zunächst inhibiert, beispielsweise mit einem Überschuß von 4-Amidinophenylbrenztraubensäure (APPA). Nach Aufkonzentrierung, bevorzugt in der Größenordnung von 1 bis 10 mg/ml, insbesondere 3 bis 5 mg/ml, beispielsweise in einem 8 mM 2-(N-Morpholino)ethansulfonsäurepuffer, wird das Protein beispielsweise gegen 0,2M  
30 3-(N-morpholino)propansulfonsäure in Ammoniumsulfat äquilibriert. Geeignete Kristalle werden durch Tropfen-Dampfdiffusion (vorzugsweise durch hanging oder sitting-drop vapour diffusion) erhalten. Tryptase-Kristalle können insbesondere durch Röntgenstrukturanalyse hinsichtlich ihrer Geometrie analysiert werden. Die dadurch erhaltenen Daten können unmittelbar zur Entwicklung von geeigneten Tryptase-Inhibitoren herangezogen werden. Deshalb umfasst die  
35 Erfindung auch ein Verfahren zur Entwicklung und/oder Identifizierung von Tryptase-Inhibitoren, welches dadurch gekennzeichnet ist, dass man anhand der Kristallstrukturdaten von kristallisierter Tryptase die Struktur des Inhibitors festlegt. Dies bedeutet insbesondere, dass man anhand der Kristallstrukturdaten von kristallisierter Tryptase die Struktur möglicher Inhibitoren

modelliert. Auf diese Weise können insbesondere bi- oder multifunktionelle Inhibitoren entwickelt werden, die eine hohe Wirksamkeit und eine hohe Spezifität für Tryptase aufweisen. Es ist aber auch möglich, monofunktionelle Inhibitoren zu entwickeln. Mit dem erfindungsgemäßen Verfahren können Verbindungen entwickelt werden, die Tryptase hemmen, ohne auf aufwendige "trial and error" Versuche angewiesen zu sein.

Die Erfindung betrifft weiterhin eine pharmazeutische Zusammensetzung, umfassend einen wie oben beschriebenen Tryptaseinhibitor. Eine solche pharmazeutische Zusammensetzung kann gegebenenfalls übliche pharmazeutische Träger oder/und Hilfsstoffe umfassen. Aufgrund des Zusammenhangs von Tryptase und einer Vielzahl von allergischen und entzündlichen Erkrankungen, wie insbesondere Asthma, Psoriasis, Arthritis, Gingivitis, Peridontitis, Rhinitis, Konjunktivitis, Dermatitis, Anaphylaxis, rheumatische Arthritis, ARDS (adult respiratory distress syndrome), Entzündungen im Magen-Darm-Bereich (Morbus Crohn, Inflammatory Bowel Disease) und anderen finden die erfindungsgemäßen pharmazeutischen Zusammensetzungen breite Anwendung. Der Tryptaseinhibitor liegt dabei in einer therapeutisch wirksamen Menge vor. Die pharmazeutische Zusammensetzung kann in allen üblichen Anwendungsformen verwendet werden. Bevorzugt liegt sie in einer Applikationsform zur topischen Anwendung vor. Beispiele hierfür sind die Verwendung als Aerosol oder als Salbe. Es ist aber auch möglich, die erfindungsgemäßen pharmazeutischen Zusammensetzungen zur oralen oder subkutanen Verabreichung bereitzustellen. Geeignete Trägerstoffe hierfür sind dem Fachmann bekannt und umfassen beispielsweise übliche Tablettierhilfsstoffe bzw. physiologische Salzlösungen.

Die Dosierung der Wirkstoffe bei systemischer Therapie. (p. o. oder i. v) liegt zwischen 0,1 und 10 mg pro Kilogramm und Tag.

Aufgrund der hohen Spezifität, die mit den erfindungsgemäßen bifunktionellen Inhibitoren erzielbar ist, eignen sie sich auch zur Diagnose von mit Tryptase in Zusammenhang stehenden Erkrankungen. Ein weiterer Gegenstand der Erfindung ist deshalb die Verwendung eines erfindungsgemäßen Tryptaseinhibitors zur Diagnose, insbesondere von allergischen und entzündlichen Erkrankungen. Daneben ist es auch möglich, mit den erfindungsgemäßen Tryptaseinhibitoren den Wirkungsmechanismus von Tryptase im einzelnen zu untersuchen und aufzuklären.

Die Erfindung wird durch die beigefügten Figuren und die nachfolgenden Beispiele weiter erläutert.

Figur 1 zeigt eine schematische Darstellung der tetrameren Struktur von Tryptase in Form eines Schnitts (11).

Die Tryptase (11) besitzt eine rahmenförmige Gestalt, in der vier strukturell identische Untereinheiten (Monomere) A (7), B (9), C (10) und D (8) die Ecken besetzen und gemeinsam einen zentralen Hohlraum (12) umschließen. Die Untereinheiten bilden in ihren aktiven Zentren

5 Spezifitätstaschen (6) aus. Bestandteil der Spezifitätstaschen (6) sind Asp189 Reste (5) der jeweiligen Untereinheiten. Die Abstände [(13)-(18)] zwischen den Carboxylgruppen der Asp189 Reste (5) in den jeweiligen Untereinheiten betragen

|    |                           |                                    |          |
|----|---------------------------|------------------------------------|----------|
|    | zwischen A (7) und B (9)  | $45 \text{ \AA} \pm 1 \text{ \AA}$ | (13),    |
| 10 | zwischen A (7) und C (10) | $45 \text{ \AA} \pm 1 \text{ \AA}$ | (14),    |
|    | zwischen A (7) und D (8)  | $33 \text{ \AA} \pm 1 \text{ \AA}$ | (15),    |
|    | zwischen B (9) und C (10) | $33 \text{ \AA} \pm 1 \text{ \AA}$ | (16),    |
|    | zwischen B (9) und D (8)  | $45 \text{ \AA} \pm 1 \text{ \AA}$ | (17) und |
|    | zwischen C (10) und D (8) | $45 \text{ \AA} \pm 1 \text{ \AA}$ | (18).    |

15

Schematisch dargestellt ist auch ein Tryptase-Inhibitor 1 dessen Kopfgruppen K1 (2) und K2 (3) mit den Carboxylgruppen der Asp189 Reste (5) in den Spezifitätstaschen (6) der Untereinheiten A (7) und D (8) der Tryptase (11) wechselwirken. Der Linker L (4) liegt in dem von den vier Untereinheiten umschlossenen Hohlraum (12).

20

Figur 2a zeigt eine Frontansicht einer Oberflächendarstellung eines festen Tryptasetetramers.

Die vier Untereinheiten (als A bis D bezeichnet) stehen durch drei zweifache Symmetrieachsen miteinander in Beziehung: zwei senkrecht zueinander entlang den Grenzflächen A-B/C-D und

25 A-D/B-C, die in der Papierebene liegen, die dritte senkrecht zu den anderen zweien, durch die Mitte des Tetramers. Die zentrale, langgestreckte Pore von Tryptase ist deutlich sichtbar. Kleine Vorsprünge von jeder der Untereinheiten verdecken teilweise den Eingang zu dieser Pore. Das elektrostatische Potential der Oberfläche ist durch + (positiv geladene Bereiche) und - (negativ geladene Bereiche) dargestellt (in der beigefügten farbigen Abbildung stellt dar: blau positiv

30 geladene Bereiche und rot negativ geladene Bereiche dar). Der an den aktiven Stellen jeder Untereinheit gelegene Inhibitor 4-Amidinophenylbrenztraubensäure (APPA) ist mit I bezeichnet (in Farbe: gelb-grün).

Figur 2b zeigt die Seitenansicht der Einheiten D und C. Ein schräger, langgestreckter Fleck mit

35 positivem Potential ( + bzw. blau) bildet eine mögliche, 108 Å lange Heparin-Bindestelle, die den Kontaktbereich zwischen den beiden Untereinheiten überspannt. Die Länge dieses Flecks ist mit der bekannten Stabilisierungsaktivität von 5,5 kDa (18-mer) und längeren Heparinketten kompatibel. (Alter et al., Biochem. J. 248 (1987), 821-827). (Die Figur wurde mit GRASP

erzeugt (Nichols et al., Biophys. J. 64 (1993) A166)).

Figur 3 zeigt eine Stereo-Banddarstellung eines Trypsasemonomers (A in Standardorientierung) mit Sekundärstrukturelementen und dem APPA-Molekül. Die Reste der aktiven Stelle sind hervorgehoben sowie die einzigartigen Oberflächenschleifen von Trypsase, nämlich (gegen den Uhrzeigersinn aufgelistet) die 37er-Schleife, die 60er-Schleife, die 97er-Schleife, 173er-Schleife, die 147er-Schleife und die 70 bis 80er-Schleife (die Figur wurde mit SETOR hergestellt (S.V. Evans, J. Mol. Graphics 11 (1990), 134-138)).

Figur 4 stellt einen Aminosäuresequenz-Vergleich auf Grundlage der Struktur von humaner Mastzelltrypsase II/β, Rindertrypsin und Rinderchymotrypsinogen A dar. Sequenzidentität und Homologie sind in gelb bzw. grün dargestellt. Eine Nummerierung auf Grundlage der Trypsase ist oberhalb der Sequenzen und eine Nummerierung auf Grundlage von Chymotrypsinogen (wie sie hierin oben verwendet wurde) ist unterhalb der Sequenzen angegeben. Die katalytischen Reste sind durch offene Dreiecke markiert und die Disulfidbrücken bildenden Cysteine durch ausgefüllte Dreiecke. Sekundäre Strukturelemente der Trypsase sind schematisch dargestellt (α1-α2 stellt α-Helizes dar, β1 bis β12 β-Stränge). (Die Figur wurde mit ALSCRIPT hergestellt (G. J. Barton, Protein Eng. 6 (1993), 37-40)).

Figur 5 stellt die Kontaktbereiche zwischen den Monomeren A und B (5a) bzw. A und C (5b) dar.

Figur 6 zeigt die finale 3 Å Elektronendichte um die Spezifitätstasche des APPA-Trypsase-Komplexes dar.

25

Figur 7 stellt die experimentelle Struktur des Trypsase-Tetramers mit einem am Monomer angedockten LDTI-Molekül dar.

Figuren 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18 und 19 zeigen Formelschemata für die Herstellung von erfindungsgemäßen bifunktionellen Inhibitoren.

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Figur 20 zeigt die aus der Röntgenstrukturanalyse gewonnenen räumlichen Koordinaten der Atome der humanen β-Trypsase (EC 3.4.21.59) im Brookhaven PDB-Format.

## Beispiele

### Beispiel 1: Proteinreinigung und Kristallisation

5

Tryptase wurde von humanem Lungengewebe bis zur offensichtlichen Homogenität unter Verwendung von bekannten Verfahren aufgereinigt (Schwartz et al., J. Biol. Chem. 256 (1981), 11939-11943; Smith et al., J. Biol. Chem. 259 (1984), 11046 bis 11051; Harvima et al., Biochim. Biophys. Acta 957 (1988), 71-80). Das Protein wurde mit einem Überschuss von 4-Amidinophenylbrenztraubensäure (APPA) inhibiert, auf 4 mg/ml in 8 mM 2-(N-Morpholino)ethansulfonsäurepuffer, pH 6,1, 1,7M Natriumchlorid konzentriert und bei 4°C gegen 0,2M 3-(N-Morpholino)propansulfonsäurepuffer, pH 5,0 und 3M Ammoniumsulfat äquilibriert. Zur Diffraktionsanalyse geeignete Kristalle wurden durch Dampfdiffusion eines sitzenden Tropfens erhalten. Die Kristalle zeigen die tetragonale Raumgruppe  $P4_1$ , haben Zellachsen  $a = b = 83 \text{ \AA}$ ,  $c = 173 \text{ \AA}$ , insbesondere  $a = b = 82,93 \text{ \AA}$ ,  $c = 172,86 \text{ \AA}$  und enthalten ein Tetramer pro asymmetrischer Einheit.

### Beispiel 2: Kristallographische Verfahren und Daten

Daten mit einer Auflösung von  $2,7 \text{ \AA}$  wurden auf einem 300 mm MAR Research image plate detector unter Verwendung von monochromatischer  $\text{CuK}\alpha$ -Strahlung von einem rotierenden Anodenröntgenstrahlgenerator (Rigaku) gesammelt. Die Datenintegration und Reduktion der Intensitäten wurde mit DENZO/SCALEPACK durchgeführt (Otwinowski et al., "DENZO: a film processing for macromolecular crystallography, Yale University, New Haven (1993) und die Umwandlung auf Strukturfaktoramplituden mit TRUNCATE (French et al, Acta Cryst. 21 (1978), 517-525). Die Struktur wurde durch molekulare Ersetzungsverfahren (molecular replacement methods) unter Verwendung von AMoRe gelöst (Navaza, Acta Cryst. A50 (1994), 157-163), unter Verwendung eines reduzierten Modells von Schweinepankreaselastase als Suchmodell. Der Modellbau wurde auf einer SGI-Graphic Workstation unter Verwendung von TurboFRODO durchgeführt (Roussel et al., TurboFRODO in Silicon Graphics geometry, Silicon Graphics, Mountain View, CA (1989).) Die kristallographische Verfeinerung und Berechnungen der Elektronendichte wurden mit X-PLOR und CCP4 durchgeführt (A.T. Brünger, XPLOR Manual, Version 3.1, Yale University, New Haven, CT (1992); Collaborative Computational Project No. 4 (1994), Acta Cryst. D50, 760-763. Das endgültige Modell hatte einen R-Faktor von 19,6 % ( $R_{\text{free}} = 28,6 \%$ ) mit einer r.m.s. Abweichung von den Zielwerten von  $0,007 \text{ \AA}$  und  $1,741^\circ$  für Bindungslängen bzw. Winkel.

**Beispiel 3: Aminosäuresequenz**

Die Aminosäuresequenz von humaner  $\beta$ -Tryptase (d.h. Tryptase II; EC 3.4.21.59), wie sie in den EMBL/PIR-Datensätzen (Eintragungen M37488/B35863 bzw. M33492/P20231) vorliegt, wurde verwendet. Diese Sequenz wurde durch Spaltung des Kristallisationsmaterials mit Trypsin und massenspektrometrischer Analyse der resultierenden Fragmente bestätigt. Die Aminosäurenummerierung folgt der des Chymotrypsinogens (vgl. Figur 4).

**Herstellung bifunktionaler Tryptase-Inhibitoren (Beispiel 4 - 14)**

10

**Beispiel 4:**

ENDPRODUKT:

**Pyridin-2,6-dicarbonsäure-bis-[4-(3-aminomethyl-benzoyl)-1-piperazid] (1)** (vgl. Fig. 8)

15

Zu einer Lösung von 600 mg (780  $\mu$ mol) Pyridin-2,6-dicarbonsäure-bis-[4-(3-butyloxycarbonyl-aminomethyl-benzoyl)-1-piperazid] in 7 ml Dioxan tropft man 1,3 ml einer 4,8 N Lösung von HCl in Dioxan (6,2 mmol). Die dicke Suspension wird mit 10 ml Methanol versetzt und 2,5 Std. gerührt. Man engt ein, nimmt in 25 ml Wasser auf und stellt die Lösung auf pH = 11 (NaOH). Man extrahiert mit 3 x 20 ml Dichlormethan, trocknet die vereinigten organischen Phasen über  $MgSO_4$  und engt ein. Das Produkt wird in 2 ml Dioxan gelöst, mit 0,5 ml einer 4,8 N Lösung von HCl in Dioxan (2,4 mmol) versetzt und die Suspension mit 15 ml Diethylether verdünnt. Die Titelverbindung wird als Hydrochlorid vom Schmp. > 260 °C isoliert.

25 AUSGANGSVERBINDUNGEN:

**Pyridin-2,6-dicarbonsäure-bis-[4-(3-tert-butyloxycarbonyl-aminomethyl-benzoyl)-1-piperazid] (2)**

Zu einer Suspension von 500 mg (1,21 mmol) Pyridin-2,6-dicarbonsäure-bis-piperazid-trihydrochlorid in 15 ml DMF gibt man nacheinander 1,36 ml (9,7 mmol) Triethylamin, 610 mg (2,42 mmol) 3-tert-Butyloxycarbonylaminomethyl-benzoesäure, 330 mg (2,42 mmol) 1-Hydroxybenzotriazol und 460 mg (2,42 mmol) N-(3-Dimethylaminopropyl)-N'-ethyl-carbodiimid-hydrochlorid (EDC x HCl). Nach 75 min wird das Reaktionsgemisch weitgehend eingeeengt, mit 20 ml Wasser versetzt und auf pH = 11 gestellt (NaOH). Man extrahiert mit 3 x 20 ml Dichlormethan, trocknet die vereinigten organischen Phasen über  $MgSO_4$ , engt ein und chromatographiert das Rohprodukt über Kieselgel (Ethylacetat/Methanol = 10:1). Das Eluat wird eingeeengt und in Diethylether ausgerührt. Man erhält 700 mg (75 %) der Titelverbindung vom Schmp. 195 °C (Aufschäumen bei 110 °C).

35

**Pyridin-2,6-dicarbonsäure-bis-piperazid (3)**

5 Zu einer Suspension von 2,05 g (4,07 mmol) Pyridin-2,6-dicarbonsäure-bis-4-tert-butyloxy-carbonyl-piperazid in 20 ml Dioxan werden 6,8 ml einer 4,8 N Lösung von HCl in Dioxan (16,2 mmol) zugetropft. Man verdünnt die Suspension mit 10 ml Methanol und rührt bei Raumtemperatur über Nacht. Das Lösungsmittel wird weitgehend eingeeengt, die Suspension mit Diethylether ausgerührt und unter Schutzgasatmosphäre filtriert. Man erhält 1,7 g (100 %) des Trihydrochlorids der Titelverbindung. Schmp. > 260 °C.

10

**Pyridin-2,6-dicarbonsäure-bis-4-tert-butyloxycarbonyl-piperazid (4)**

1,0 g (5,0 mmol) 2,6-Pyridindicarbonyldichlorid in 10 ml Dioxan werden zu einer Lösung von 1,88 g (10,1 mmol) Piperazin-N-carbonsäure-tert-butylester in 0,82 ml (10,1 mmol) Pyridin, 15 3,5 ml (25,2 mmol) Triethylamin und 10 ml Dioxan getropft. Man rührt bei Raumtemperatur über Nacht, filtriert vom Niederschlag ab und engt die Mutterlauge zur Trockne ein. Der Rückstand wird mit 3 x 30 ml Dichlormethan aus 30 ml Wasser extrahiert. Die über MgSO<sub>4</sub> getrocknete organische Phase wird eingeeengt und aus Diethylether kristallisiert. Man erhält 2,16 g (90 %) der Titelverbindung vom Schmp. 183-186 °C.

20

**Beispiel 5:****ENDPRODUKTE**

25 **Pyridin-2,6-dicarbonsäure-bis-[4-(trans-4-aminomethylcyclohexanoyl)-1-piperazid] (5)**  
(vgl. Fig. 9)

Zu einer Lösung von 500 mg (640 µmol) Pyridin-2,6-dicarbonsäure-bis-[4-(trans-4-tert-butyloxy-carbonylaminomethylcyclohexylcarbonyl)-1-piperazid] in 10 ml Dioxan tropft man 1,06 ml einer 30 4,6 N Lösung von HCl in Dioxan (5,1 mmol). Die dicke Suspension wird mit 20 ml Methanol versetzt und 4 Std. bei 40 °C gerührt. Man engt ein, koevaporiert mit 2 x 20 ml Toluol und kristallisiert den Rückstand aus Diethylether. Die Titelverbindung wird als Dihydrochlorid vom Schmp. 170 °C (Aufschäumen) isoliert.

35 **2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-[4-(3-aminomethyl-benzoyl)-1-piperazid] (7)** (vgl. Fig. 10)

Zu einer Lösung von 350 mg (0,4 mmol) 2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-

[4-(3-tert-butyloxycarbonyl-aminomethyl-benzoyl)-1-piperazid] in 5 ml Dioxan und 5 ml Methanol gibt man 522 µl einer 4,6 N Lösung von HCl in Dioxan (2,4 mmol). Nach Rühren über Nacht bei Raumtemperatur werden nochmals 200 µl (0,9 mmol) HCl in Dioxan zugegeben und das Reaktionsgemisch 5 Std. auf 40 °C erhitzt. Man engt ein, verrührt den Rückstand mit 5 ml Dioxan und 2 ml Diethylether und isoliert die Titelverbindung als Dihydrochlorid vom Schmp. 250 °C (Sintern bei 223 °C).

#### AUSGANGSVERBINDUNGEN:

#### 10 Pyridin-2,6-dicarbonsäure-bis-[4-(trans-4-tert-butyloxycarbonyl-aminomethylcyclohexyl-carbonyl)-1-piperazid] (6)

Zu einer Suspension von 500 mg (1,21 mmol) Pyridin-2,6-dicarbonsäure-bis-piperazid-trihydrochlorid in 15 ml DMF gibt man nacheinander 1,36 ml (9,7 mmol) Triethylamin, 620 mg (2,42 mmol) trans-4-tert-Butyloxycarbonyl-aminomethylcyclohexancarbonsäure, 330 mg (2,42 mmol) 1-Hydroxybenzotriazol und 460 mg (2,42 mmol) N-(3-Dimethylaminopropyl)-N'-ethyl-carbodiimid-hydrochlorid (EDC x HCl). Nach 45 min wird das Reaktionsgemisch weitgehend eingengt, mit 20 ml Wasser versetzt und auf pH = 12 gestellt (NaOH). Man extrahiert mit 3 x 20 ml Dichlormethan, trocknet die vereinigten organischen Phasen über MgSO<sub>4</sub>, engt ein und chromatographiert das Rohprodukt über Kieselgel (Ethylacetat/Methanol/Ammoniak = 10:1:0,5). Das Eluat wird eingengt und in Diisopropylether ausgerührt. Man erhält 620 mg (65 %) der Titelverbindung vom Schmp. 200-202 °C.

#### 25 2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-[4-(3-tert-butyloxycarbonyl-aminomethylbenzoyl)-1-piperazid] (8)

Zu einer Suspension von 220 mg (0,53 mmol) 2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-piperazid in 10 ml DMF gibt man nacheinander 500 µl (4,2 mmol) Triethylamin, 280 mg (1,1 mmol) 3-tert-Butyloxycarbonylaminomethyl-benzoesäure, 280 mg (1,1 mmol) 1-Hydroxybenzotriazol und 280 mg (2,1 mmol) N-(3-Dimethylaminopropyl)-N'-ethyl-carbodiimid-hydrochlorid (EDC x HCl). Nach 4 Std. wird das Reaktionsgemisch weitgehend eingengt, mit 30 ml Wasser versetzt und auf pH = 12 gestellt (NaOH). Man extrahiert mit insgesamt 70 ml Dichlormethan, trocknet die vereinigten organischen Phasen über MgSO<sub>4</sub>, engt ein und chromatographiert das Rohprodukt über Kieselgel (Ethylacetat/Methanol = 10:1). Das Eluat wird eingengt und der Rückstand in Diisopropylether ausgerührt. Man erhält 446 mg (96 %) der Titelverbindung vom Schmp. 113 °C.

**2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-piperazid (9)**

- 5 Zu einer Suspension von 5,87 g (9,6 mmol) 2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-4-tert-butyloxycarbonyl-piperazid in 20 ml Dioxan und 10 ml Methanol werden 12,6 ml einer 4,6 N Lösung von HCl in Dioxan (57,6 mmol) zugetropft. Man rührt 5 Std. bei Raumtemperatur. Das Lösungsmittel wird eingeeengt und der Rückstand mit 30 ml Diethylether und 70 ml Methanol ausgerührt. Man erhält 4,35 g (94 %) des Dihydrochlorids der Titelverbindung vom Schmp. > 250 °C.

10 **2,6-Dimethyl-4-phenyl-pyridin-3,5-dicarbonsäure-bis-4-tert-butyloxycarbonyl-piperazid (10)**

- 15 13,0 g (mmol) Dikalium-2,6-dimethyl-4-phenyl-pyridin-3,5-dicarboxylat werden in 80 ml Phosphoroxychlorid unter Stickstoffatmosphäre 5 Std. bei 100 °C gekocht. Das Phosphoroxychlorid wird im Vakuum abdestilliert und der Rückstand mit 3 x 50 ml Toluol koevaporiert. Zu einer Lösung von 12,8 g (66 mmol) Piperazin-N-Carbonsäure-tert-butylester, 5,3 ml (66 mmol) Pyridin und 46 ml (450 mmol) Triethylamin in 100 ml Dioxan tropft man unter Temperaturkontrolle (< 30 °C) eine Suspension des rohen Säurechlorids in 200 ml Dioxan. Nach einer Stunde werden die anorganischen Salze abfiltriert und das Filtrat eingeeengt. Der Rückstand wird mit 3 x 20 70 ml Ethylacetat aus 100 ml Wasser extrahiert. Die über MgSO<sub>4</sub> getrockneten vereinigten organischen Phasen werden eingeeengt und über Kieselgel chromatographiert (Ethylacetat/Methanol = 10:1). Man erhält 7,13 g (35 %) der Titelverbindung als gelbliches Öl.

**Beispiel 6:**

25

ENDPRODUKT:

**Pyridin-2,6-dicarbonsäure-bis-[4-(3-aminomethyl-benzoylamino)-1-piperidid] (11)**

(vgl. Fig. 11)

- 30 Zu einer Lösung von 220 mg (275 µmol) Pyridin-2,6-dicarbonsäure-bis-[4-(3-tert-butyloxycarbonyl-aminomethyl-benzoylamino)-1-piperidid] in 5 ml Dioxan tropft man 275 µl einer 4 N Lösung von HCl in Dioxan (1,1 mmol). Die dicke Suspension wird mit 3 ml Methanol versetzt und 12 Std. gerührt. Man engt ein, koevaporiert mit 2 x 20 ml Toluol und kristallisiert. Man erhält 130 mg der Titelverbindung vom Schmp. 230° C (Aufschäumen).

35

## AUSGANGSVERBINDUNGEN:

**Pyridin-2,6-dicarbonsäure-bis-[4-(3-tert-butyloxycarbonyl-aminomethyl-benzoyl-amino)-1-piperidid] (12)**

- 5 Zu einer Suspension von 250 mg (0,62 mmol) Pyridin-2,6-dicarbonsäure-bis-(4-amino-1-piperidid) Dihydrochlorid in 2,5 ml DMF und 2,5 ml Dioxan gibt man nacheinander 342 mg (1,36 mmol) 3-tert-Butyloxycarbonylaminomethyl-benzoesäure, 240 µl (1,36 mmol) Hünig Base, 30 mg Diaminopyridin und 260 mg (1,36 mmol) N-(3-Dimethylaminopropyl)-N'-ethyl-carbodiimid-hydrochlorid (EDC x HCl). Nach 12 Std. Rühren bei Raumtemp. wird das
- 10 Reaktionsgemisch eingeeengt, mit 10 ml Wasser versetzt und auf pH = 3 gestellt (0,1 N HCl). Man extrahiert mit 3 x 20 ml Dichlormethan, trocknet die vereinigten organischen Phasen über MgSO<sub>4</sub>, engt ein und chromatographiert das Rohprodukt über Kieselgel (Dichlormethan/Methanol = 19:1). Das produkthaltige Eluat wird eingeeengt und in Diethyl-ether ausgerührt. Man erhält 280 mg (57%) der Titelverbindung vom Schmp. 140°C (Aufschäumen, Sintern ab 120°C).
- 15

**Pyridin-2,6-dicarbonsäure-bis-(4-amino-1-piperidid) (13)**

- Zu einer Lösung von 2,0 g (3,76 mmol) Pyridin-2,6-dicarbonsäure-bis-4-tert-butyloxycarbonylamino-1-piperidid in 10 ml Diethylether, 30 ml Methanol und 20 ml Dichlormethan tropft man 12 ml einer 6 N Lösung von HCl in Diethylether (72 mmol) und erhitzt das Reaktionsgemisch 2 Std. auf 40° C. Das Lösungsmittel wird eingeeengt, der Rückstand mit Diethylether ausgerührt und unter Schutzgasatmosphäre abfiltriert. Man erhält 1,52 g (100%) des Dihydrochlorids der Titelverbindung. Schmp. 130°C.
- 20

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**Pyridin-2,6-dicarbonsäure-bis-4-tert-butyloxycarbonylamino-1-piperidid (14)**

- 850 mg (4,05 mmol) 2,6-Pyridindicarbonyldichlorid in 10 ml Dioxan werden zu einer Suspension von 1,67 g (8,08 mmol) Piperidin-N-carbonsäure-tert-butylester in 0,65 ml (8,08 mmol) Pyridin, 2,8 ml (20 mmol) Triethylamin und 10 ml Dioxan getropft. Man rührt bei Raumtemp. über Nacht und engt ein. Der Rückstand wird mit 30 ml Wasser versetzt und mit NaOH basisch gestellt (pH = 11). Man extrahiert mit 3 x 30 ml Dichlormethan, trocknet die vereinigten organischen Phasen über MgSO<sub>4</sub>, engt ein und kristallisiert aus Diethylether. Man erhält 2,12 g (99%) der Titelverbindung vom Schmp. 90°C.
- 30

35

**Beispiel 7:**

ENDPRODUKT:

**Pyridin-2,6-dicarbonsäure-bis-[4-(4-aminomethyl-cyclohexylcarbonylamino)-1-piperidid]**5 **(15)** (vgl. Figur 12)

Zu einer Suspension von 160 mg (197 µmol) Pyridin-2,6-dicarbonsäure-bis-[4-(4-tert-butyl-oxycarbonyl-aminomethyl-cyclohexylcarbonyl-amino)-1-piperidid] in 10 ml Dioxan und 2 ml Methanol tropft man 500 µl einer 4 N Lösung von HCl in Dioxan (2,0 mmol) und rührt 12 Std. bei Raumtemp. Man engt ein, koevaporiert zweimal mit 50 ml Diethylether und rührt das Rohprodukt in Diethylether aus. Man erhält 100 mg der Titelverbindung vom Schmp. >250°C.

AUSGANGSVERBINDUNGEN:

15 **Pyridin-2,6-dicarbonsäure-bis-[4-(4-tert-butyloxycarbonyl-aminomethyl-cyclohexyl-carbonyl-amino)-1-piperidid] (16)**

Zu einer Suspension von 250 mg (0,62 mmol) Pyridin-2,6-dicarbonsäure-bis-(4-amino-1-piperidid) Dihydrochlorid in 2,5 ml DMF und 2,5 ml Dioxan gibt man nacheinander 350 mg (1,36 mmol) trans-3-tert-Butyloxycarbonylaminomethyl-cyclohexylcarbonsäure, 240 µl (1,36 mmol) Hünig Base, 30 mg Diaminopyridin und 260 mg (1,36 mmol) N-(3-Dimethylaminopropyl)-N'-ethyl-carbodiimid-hydrochlorid (EDC x HCl). Nach 12 Std. Rühren bei Raumtemp. wird das Reaktionsgemisch eingeeengt, mit 10 ml Wasser versetzt und auf pH = 3 gestellt (0,1 N HCl). Man extrahiert mit 3 x 20 ml Dichlormethan, trocknet die vereinigten organischen Phasen über MgSO<sub>4</sub>, engt ein und chromatographiert das Rohprodukt über Kieselgel (Dichlormethan/Methanol = 19:1). Das produktthaltige Eluat wird eingeeengt und in Diethylether ausgerührt. Man erhält 230 mg (46%) der Titelverbindung vom Schmp. > 250°C.

**Beispiel 8:**

30 ENDPRODUKT:

**Bis{4-[4-(4-aminomethyl)cyclohexanoyl]piperazin-1-yl}carbonyl}4,4'-diamino-diphenyl-ether Dihydrochlorid (17)** (vgl. Fig. 13)

Bis{4-[4-(4-tert-butoxycarbonyl-aminomethyl)cyclohexanoyl-piperazin-1-yl]carbonyl}4,4'-diamino-diphenylether (0,18 g; 0,2 mmol) wird in 4,8 M HCl in Dioxan (5 ml) suspendiert. Die Suspension wird 24 Stunden bei 40 – 45°C gerührt. Nach Zugabe von Diethylether (25 ml) wird im Eisbad gekühlt. Das ausgefallene Produkt wird abgenutscht, mehrmals mit Diethylether gewaschen und im Vakuum getrocknet. Ausbeute: 0,12 g, weisser amorpher Feststoff.

MS (ESI): 703,4 (100) MH<sup>+</sup>

AUSGANGSVERBINDUNGEN:

Bis[4-[4-(4-tert-butoxycarbonyl-aminomethyl)cyclohexanoyl-piperazin-1-yl]carbonyl]-

5 4,4'-diamino-diphenylether (18)

4,4'-Bis(1-piperazinylcarbonyl)diphenylether-dihydrochlorid (0,25 g; 0,5 mmol), Boc-trans-  
examsäure (0,28 g; 1,1 mmol), N-Ethyl-diisopropylamin (0,2 ml; 1,1 mmol) und 4-Dimethyl-  
aminopyridin (5 mg) werden in Dimethylformamid (2,5 ml) und Dichlormethan (2,5 ml) 15  
10 Minuten bei Raumtemperatur gerührt. Nach Zugabe von N-(3-Dimethylaminopropyl)-N'-  
ethylcarbodiimid-hydrochlorid (0,21 g; 1,1 mmol) wird das Reaktionsgemisch 24 Stunden bei  
40°C gerührt. Das Lösungsmittel wird im Vakuum vollständig abgezogen. Der Rückstand  
wird an Kieselgel chromatographiert (Dichlormethan : Methanol – 9 : 1). Die Produktfraktion  
wird gesammelt und das Lösungsmittel vollständig im Vakuum abgezogen. Ausbeute: 0,18 g,  
15 weisser amorpher Feststoff.

MS (ESI): 903,1 (100) MH<sup>+</sup>

4,4'-Bis(1-piperazinylcarbonyl)diphenylether Dihydrochlorid (19)

20 4,4'-Bis[4-(tert-butoxycarbonyl)-1-piperazinylcarbonyl]diphenylether (6,4 g; 10,2 mmol)  
wird in 4,8 M HCl in Dioxan (50 ml) suspendiert. Die Suspension wird 22 Stunden bei  
40-45°C gerührt. Nach Zugabe von Diethylether (100 ml) wird im Eisbad gekühlt. Das  
ausgefallene Produkt wird abgenutscht, mehrmals mit Diethylether gewaschen und im  
Vakuum getrocknet. Ausbeute: 4,65 g, weisser amorpher Feststoff.  
25 MS(APCI): 425,0 (100) MH<sup>+</sup>

4,4'-Bis[4-(tert-butoxycarbonyl)-1-piperazinylcarbonyl]diphenylether (20)

Zur gerührten Lösung von 1-tert.-Butoxycarbonylpiperazin (4,10 g; 22 mmol) in Dichlormethan  
30 (50 ml) wird bei Raumtemperatur eine Lösung von Oxy-bis-(4-phenyl-isocyanat) (2,52 g,  
10 mmol) in Dichlormethan (25 ml) zugetropft. Nach beendeter Zugabe wird weitere drei  
Stunden bei Raumtemperatur gerührt. Das ausgefallene Produkt wird abgenutscht, mehrmals  
mit Hexan gewaschen und in Vakuum getrocknet. Ausbeute: 6,20 g weisser amorpher  
Feststoff.  
35 MS(EI): 625,5 (12) MH<sup>+</sup>; 271,2 (26); 118,2 (42); 187,1 (100)

**Beispiel 9:**

ENDPRODUKT:

**Bis{4-[4-(3-aminomethyl)benzoyl-piperazin-1-yl]carbonyl}4,4'-diamino-diphenylether**5 **Dihydrochlorid (21)** (vgl. Fig. 14)

Bis{4-[4-(3-tert-butoxycarbonyl-aminomethyl)benzoyl-piperazin-1-yl]carbonyl}4,4'-diamino-diphenylether (0,31 g; 0,35 mmol) wird in 4,8 M HCl in Dioxan (5 ml) 24 Stunden bei 40 - 45°C gerührt. Nach Zugabe von Diethylether (25 ml) wird im Eisbad gekühlt. Das  
10 ausgefallene Produkt wird abgenutscht, mehrmals mit Diethylether gewaschen und im Vakuum getrocknet. Ausbeute: 0,19 g, weisser amorpher Feststoff.

MS (ESI): 691.2 (100) MH<sup>+</sup>

AUSGANGSVERBINDUNGEN:

15 **Bis{4-[4-(3-tert-butoxycarbonyl-aminomethyl)benzoyl-piperazin-1-yl]carbonyl}4,4'-diamino-diphenylether (22)**

4,4'-Bis(1-piperazinylcarbonyl)diphenylether Dihydrochlorid (0,25 g; 0,5 mmol), 3-(tert-butoxycarbonylaminomethyl)benzoesäure (0,28 g; 1,1 mmol), N-Ethyl-diisopropylamin (0,2 ml; 1,1 mmol) und 4-Dimethylaminopyridin (30 mg) werden in Dimethylformamid (2,5 ml) und  
20 Dioxan (2,5 ml) 15 Minuten bei Raumtemperatur gerührt. Nach Zugabe von N-(3-Dimethylaminopropyl)-N'-ethylcarbodiimid-hydrochlorid (0,21 g; 1,1 mmol) wird das Reaktionsgemisch 24 Stunden bei Raumtemperatur gerührt. Das Lösungsmittel wird im Vakuum vollständig abgezogen. Der Rückstand wird an Kieselgel chromatographiert (Dichlormethan :  
25 Methanol – 9 : 1). Die Produktfraktion wird gesammelt und das Lösungsmittel vollständig im Vakuum abgezogen. Ausbeute: 0,32 g, viskoses Öl.

MS (ESI): 890.8, M<sup>+</sup>; 791.2, MH-Boc<sup>+</sup>**Beispiel 10:**

30

ENDPRODUKT:

**Di{4-[4-(4-aminomethyl)cyclohexanoylamino]piperidin-1-yl-carbamoyl}cyclohexylmethan Dihydrochlorid (23)** (vgl. Fig. 15)

Di{4-[4-(4-tert-butoxycarbonyl-aminomethyl)cyclohexanoylamino]piperidin-1-yl-carbamoyl}-cyclohexylmethan (0,65 g; 0,7 mmol) wird in 4,8 M HCl in Dioxan (7 ml) 24 Stunden bei 40 – 45°C gerührt. Nach Zugabe von Diethylether (50 ml) wird im Eisbad gekühlt. Das ausgefallene

ne Produkt wird abgenutscht, mehrmals mit Diethylether gewaschen und im Vakuum getrocknet. Ausbeute: 0,26 g, weisser amorpher Feststoff.

MS (ESI): 741,5 (100) MH<sup>+</sup>

5 AUSGANGSVERBINDUNGEN:

**Di[4-[4-(4-tert.-butoxycarbonyl-aminomethyl)cyclohexanoylamino]piperidin-1-yl-carbamoyl]cyclohexylmethan (24)**

- 10 Di[4-(4-Amino-piperidin-1-yl-carbamoyl)]cyclohexyl-methan Dihydrochlorid (0,54 g; 1,0 mmol), Boc-tranexamsäure (0,57 g; 2,2 mmol), N-Ethyldiisopropylamin (0,38 ml; 2,2 mmol) und 4-Dimethylaminopyridin (30 mg) werden in Dimethylformamid (5 ml) und Dioxan (5 ml) 15 Minuten bei Raumtemperatur gerührt. Nach Zugabe von N-(3-Dimethylaminopropyl)-N'-ethylcarbodiimid-hydrochlorid (0,43 g; 2,2 mmol) wird das Reaktionsgemisch 48 Stunden bei 40°C gerührt. Das Lösungsmittel wird im Vakuum vollständig abgezogen. Der Rückstand wird an Kieselgel chromatographiert (Dichlormethan : Methanol; 9 : 1). Die Produktfraktion wird gesammelt und das Lösungsmittel vollständig im Vakuum abgezogen. Ausbeute: 0,65 g, viskoses Öl, das ohne Charakterisierung weiter umgesetzt wurde.

20 **Di[4-(4-Amino-piperidin-1-yl-carbamoyl)]cyclohexyl-methan Dihydrochlorid (25)**

- 25 Di[4-[4-(tert.-Butoxycarbamoyl)piperidin-1-yl-carbamoyl]]cyclohexyl-methan (4,90 g; 7,0 mmol) wird in 4,8 M HCl in Dioxan (50 ml) suspendiert. Die Suspension wird 48 Stunden bei 40 – 45°C gerührt. Nach Zugabe von Diethylether (100 ml) wird im Eisbad gekühlt. Das ausgefallene Produkt wird abgenutscht, mehrmals mit Diethylether gewaschen und im Vakuum getrocknet. Ausbeute: 4,10 g, weisser amorpher Feststoff.  
MS(EI): 463,4 (100) MH<sup>+</sup>

**Di[4-[4-(tert.-Butoxycarbamoyl)piperidin-1-yl-carbamoyl]]cyclohexyl-methan (26)**

- 30 Zur gerührten Lösung von 4-tert.-Butoxycarbamoyl-piperidin (3,20 g; 16,0 mmol) in Dichlormethan (30 ml) wird bei Raumtemperatur eine Lösung von Dicyclohexylmethan-4,4'-diisocyanat (1,90 g; 7,3 mmol) in Dichlormethan (10 ml) zugetropft. Nach beendeter Zugabe wird weitere drei Stunden bei Raumtemperatur gerührt. Das ausgefallene Produkt wird abgenutscht, mehrmals mit Hexan gewaschen und in Vakuum getrocknet. Ausbeute: 4,10 g weisser amorpher Feststoff.  
MS(ESI): 685,3 (57) MNa<sup>+</sup>; 663,2 (100) MH<sup>+</sup>

**Beispiel 11:****ENDPRODUKT:****2,2-Bis{4-[4-(4-aminophenyl)-1-piperazinylcarbonyl-methoxy]phenyl}propan** Dihydro-5 **chlorid (27)** (vgl. Fig. 16)

0,65 g 2,2-Bis{4-[4-(4-nitrophenyl)-1-piperazinylcarbonyl-methoxy]phenyl}propan werden in 60 ml Eisessig gelöst und 0,2 g Palladiumkohle (10 %) zugegeben. Das Gemisch wird in einer Umlaufapparatur hydriert bis kein Ausgangsprodukt mehr nachweisbar ist (DC). Es wird vom  
10 Katalysator über Celite abgesaugt und das Filtrat am Rotationsverdampfer im Vakuum bis zur Trocknung eingedampft. Der Rückstand wird im Dichlormethan gelöst, die Lösung mit NaHCO<sub>3</sub>-Lösung gewaschen, über Na<sub>2</sub>SO<sub>4</sub> getrocknet, filtriert und wieder eingeeengt. Der Rückstand wird  
15 über eine Kieselgelsäule mit einem Gemisch aus Ethylacetat/Methanol/NH<sub>4</sub>OH (25 %) im Verhältnis von 90:8:2 als Laufmittel chromatographiert. Die chromatographisch reinen  
Fraktionen werden vereint, eingeeengt und der Rückstand in Dichlormethan gelöst. Nach Zugabe von ätherischer Salzsäure wird eingeeengt, noch zweimal mit Dichlormethan nachdestilliert und dann der Rückstand mit Ethylacetat/Isopropanol verrieben. Der Niederschlag wird abgesaugt, gewaschen und dann im Hochvakuum getrocknet. Man erhält 0,32 g der Titelverbindung mit Schmp. ab 182 °C Zersetzung.

20

**AUSGANGSVERBINDUNGEN:****2,2-Bis{4-[4-(4-nitrophenyl)-1-piperazinylcarbonyl-methoxy]phenyl}propan (28)**

2,5 g 4-[4-Carboxylmethoxyphenyl]-1-methyl-ethyl]phenoxyessigsäure werden in Toluol suspendiert und 1,6 ml Thionylchlorid zugegeben. Das Gemisch wird 5 Stunden unter Rückfluß  
25 erhitzt und nach Abkühlen am Rotationsverdampfer eingeeengt. Es wird noch zweimal mit Toluol nachdestilliert und dann das erhaltene rohe Disäurechlorid in 50 ml abs. Dioxan gelöst. Es werden nacheinander 2,95 g 1-(4-Nitrophenyl)-piperazin, 2 ml Triethylamin und eine Spatelspitze 4-Dimethylaminopyridin zugegeben. Das Gemisch wird 2,5 h bei 50 °C gerührt. Nach  
30 Abkühlen wird mit Wasser versetzt, der pH mit verdünnter Natronlauge auf 9 eingestellt. Das abgeschiedene Produkt wird durch Anreiben zur Kristallisation gebracht, abgesaugt, mit Wasser gewaschen und über Calciumchlorid getrocknet. Man erhält 4,7 g der Titelverbindung mit Schmp. ab 165 °C Zersetzung.

35 **4-[1-(4-Carboxymethoxyphenyl)-1-methyl-ethyl]-phenoxyessigsäure (29)**

6,7 g 4-[1-(4-Ethoxycarbonylmethoxyphenyl)-1-methyl-ethyl]phenoxyessigsäure-ethylester werden in 20 ml Methanol gelöst und 16,7 g 10 %-ige Natronlauge zugegeben. Das Gemisch wird

3 Stunden unter Rückfluß zum Sieden erhitzt, abgekühlt und dann das Methanol am Rotationsverdampfer abdestilliert. Es wird mit Wasser verdünnt, mit 2 N HCl auf pH 2 angesäuert und dann der farblose Niederschlag abgesaugt, mit Wasser gewaschen und im Vakuum über Calciumchlorid getrocknet. Man erhält 5,5 g der Titelverbindung mit Schmp. 177 - 179 °C.

5

**4-[1-(4-Ethoxycarbonylmethoxyphenyl)-1-methyl-ethyl]phenoxyessigsäureethylester (30)**

Ein Gemisch aus 10 g 4,4'-Isopropylidendiphenol, 10,7 ml Bromessigsäureethylester, 15,2 g Kaliumcarbonat und 1 Spatelspitze 18-Krone-6 in 180 ml Aceton wird in 4 Stunden unter Rückfluß zum Sieden erhitzt. Dann wird vom Feststoff abgesaugt, das Filtrat im Vakuum eingeeengt und der Rückstand mit 100 ml Diisopropylether versetzt. Es wird abgesaugt, mit wenig Diisopropylether gewaschen und getrocknet. Man erhält 15,5 g der Titelverbindung mit Schmp. 69 - 71 °C.

15

**Beispiel 12:**

ENDPRODUKT:

**2,2-Bis-[4-(4-quanidiny-benzylamino)carbonylmethoxyphenyl]propan-dihydroacetat**

20 **(31)**

(vgl. Fig. 17)

0,63 g 2,2-Bis-[4-(4-aminobenzylamino)carbonylmethoxyphenyl]propan in 10 ml abs. DMF werden nacheinander unter Rühren mit 0,88 g 1,3-Bis(benzyloxycarbonyl)-2-methylisothioharnstoff, 0,68 g Quecksilber(II)chlorid und 0,69 g Triethylamin versetzt. Das Gemisch wird 3 h bei Raumtemperatur gerührt, dann wird mit Ethylacetat verdünnt, vom entstandenen Niederschlag abgesaugt und das Filtrat einmal mit 5 %iger Sodalösung und zweimal mit Wasser gewaschen. Die Lösung wird über Magnesiumsulfat getrocknet, abgesaugt und das Filtrat im Vakuum zur Trockene eingedampft. Das Öl wird über eine Kieselgelsäule mit einem Gemisch aus Dichlormethan/Ethanol 95:5 chromatografiert. Die chromatografisch reinen Fraktionen werden vereinigt, eingeeengt und der Rückstand (0,9 g) in einem Gemisch aus 60 ml Tetrahydrofuran, 3 ml Methanol und 1 ml Eisessig gelöst. Nach Zugabe von 0,3 g Palladiumkohle (10 %) wird in einer Umlaufapparatur hydriert bis kein Ausgangsprodukt mehr nachweisbar ist. Es wird vom Katalysator abgesaugt und zur Trockene eingedampft. Das verbleibende zähe Öl wird mit THF verrührt, der entstandene Niederschlag abgesaugt, mit THF und Diethylether gewaschen und in Vakuum bei 80° C getrocknet. Man erhält 0,35 g der Titelverbindung mit Schmp. 135° (Zersetzung).

35

**AUSGANGSVERBINDUNGEN:****2,2-Bis-[4-(4-aminobenzylamino)carbonylmethoxyphenyl]propan (32)**

- 5 1,8 g 2,2-Bis-[4-(4-nitrobenzylamino)carbonylmethoxyphenyl]propan werden in 300 ml THF gelöst und nach Zugabe von 0,5 g Palladiumkohle (10 %) in einer Umlaufapparatur hydriert bis kein Ausgangsprodukt mehr nachweisbar ist (DC). Nach Absaugen des Katalysators wird das Filtrat im Vakuum zur Trockene eingeeengt und der Rückstand über eine Kieselgelsäule mit einem Gemisch aus Dichlormethan/Ethanol 95:5 chromatografiert. Die chromatografisch
- 10 reinen Fraktionen werden vereint, eingeeengt und der Rückstand im Hochvakuum getrocknet. Man erhält 1,05 g der Titelverbindung in Form eines erstarrten Schaumes.

**2,2-Bis-[4-(4-nitrobenzylamino)carbonylmethoxyphenyl]propan (33)**

- 15 2 g 4-[1-(4-Carboxymethoxyphenyl)-1-methylethyl]-phenoxyessigsäure in 100 ml Toluol werden mit 1,5 ml Thionylchlorid versetzt und das Gemisch 5 h unter Rückfluß zum Sieden erhitzt. Nach Abkühlen wird am Rotationsverdampfer eingeeengt und noch zweimal mit Toluol nachdestilliert. Das so erhaltene Disäurechlorid wird in 40 ml abs. Dioxan gelöst, 2,2 g 4-
- 20 Nitrobenzylamin-hydrochlorid zugegeben und dann 3,5 ml Triethylamin zugetropft. Das Gemisch wird 2 h bei 50 °C gerührt und dann im Vakuum eingeeengt. Der nach Zugabe von Wasser entstandene Niederschlag wird abgesaugt, im Vakuum getrocknet und zur weiteren Reinigung über eine Kieselgelsäule mit Ethylacetat chromatografiert. Die chromatografisch
- 25 reinen Fraktionen werden vereint, eingeeengt und getrocknet. Man erhält 1,25 g der Titelverbindung als erstarrten Schaum.

**Beispiel 13:**

- 30 **ENDPRODUKT:**

**2,2-Bis-[4-(10-amino-3,6-diaza-2,5-dioxodecyloxy)phenyl]propan-dihydrochlorid (34)**

(vgl. Fig. 18)

- 0,77 g 2,2-Bis-[4-[10-(tert.butoxycarbonylamino)-3,6-diaza-2,5-dioxodecyloxy]phenyl]propan
- 35 werden in 10 ml abs. Dioxan gelöst und mit 2 ml einer ca. 4,8 M Lösung von Chlorwasserstoff in Dioxan versetzt. Es wird über Nacht gerührt, dann der entstandene Niederschlag abgesaugt, mit Dioxan und dann mit Diethylether gewaschen und bei 80° C im Vakuum getrocknet. Man erhält 0,58 g der Titelverbindung mit Schmp. 173° C (Zersetzung).

## AUSGANGSVERBINDUNGEN:

2,2-Bis-[4-(10-(tert.butoxycarbonylamino)-3,6-diaza-2,5-dioxodecyloxy)phenyl]propan5 (35)

0,67 g 2,2-Bis-(4-chlorcarbonylmethoxyphenyl)propan (hergestellt analog Beispiel 33) in 5 ml abs. Dioxan werden unter Rühren zu einer Lösung von 0,85 g N-[4-(tert.Butoxycarbonylamino)butyl]glycinamid und 0,42 Triethylamin in 10 ml abs. Dioxan zugetropft. Die Mischung wird über Nacht gerührt, in Vakuum eingeengt und der Rückstand zwischen Wasser und Ethylacetat verteilt. Die organische Phase wird zweimal mit Wasser gewaschen, über Magnesiumsulfat getrocknet und eingeengt. Der Rückstand wird über eine Kieselgelsäule mit einem Gemisch aus Dichlormethan/Ethanol 95:5 chromatografiert. Die chromatografisch reinen Fraktionen werden vereint, eingeengt und der Rückstand mit Diethylether/2-Propanol kristallisiert. Es wird abgesaugt, mit Diethylether gewaschen und in Vakuum getrocknet. Man erhält 0,77 g der Titelverbindung mit Schmp. 59° C (Zersetzung).

Beispiel 14:

20

## ENDPRODUKT:

2,2-Bis-[4-[4-(4-aminomethylbenzylcarbamoyl)-1-piperazinylcarbonyloxy]phenyl]-propan-dihydrochlorid (36) (vgl. Fig. 19)

25 0,14 g 2,2-Bis-[4-[4-(4-tert.butoxycarbonylaminomethylbenzylcarbamoyl)-1-piperazinylcarbonyloxy]phenyl]propan werden in 2 ml abs. Dioxan gelöst und mit 2 ml einer ca. 20%igen Chlorwasserstoff-Lösung im Dioxan versetzt. Es wird über Nacht gerührt, abgesaugt, zweimal mit Diethylether gewaschen und im Vakuum getrocknet. Man erhält 0,08 g der Titelverbindung mit Schmp. ab 250° C (Zersetzung).

30

## AUSGANGSVERBINDUNGEN:

2,2-Bis-[4-[4-(4-tert.butoxycarbonylaminomethylbenzylcarbamoyl)-1-piperazinylcarbonyloxy]phenyl]propan (37)

35

0,2 g 2,2-Bis-[4-(1-piperazinylcarbonyloxy)phenyl]propan-dihydrochlorid und 0,66 ml Diisopropylethylamin werden in 5 ml Dichlormethan gelöst und dann mit 0,4 ml einer 20%igen Phosgenlösung in Toluol versetzt. Nach 30 min Rühren bei Raumtemperatur

werden 0,18 g 4-(tert.Butoxycarbonylaminomethyl)benzylamin zugegeben und weitere 30 min. gerührt. Dann wird mit Wasser versetzt, die Phasen getrennt und die organische Phase noch zweimal mit Wasser gewaschen. Nach Trocknen über Magnesiumsulfat wird am Rotationsverdampfer eingeengt. Der Rückstand wird über eine Kieselgelsäule mit Dichlormethan/Methanol 95:5 als Laufmittel chromatografiert. Die chromatografisch reinen Fraktionen werden vereinigt und im Vakuum zur Trockene eingedampft. Man erhält 0,17 g der Titelverbindung als erstarrten Schaum.

#### **2,2-Bis-[4-(1-piperazinyloxy)phenyl]propan-dihydrochlorid (38)**

10

8,3 g 2,2-Bis-[4-(4-tert.butoxycarbonyl-1-piperazinyloxy)phenyl]propan-dihydrochlorid werden in 50 ml abs. Dioxan gelöst und unter Rühren mit 9,5 ml einer ca. 20%igen Chlorwasserstoffsäure in Dioxan versetzt. Das Gemisch wird über Nacht gerührt, mit Toluol verdünnt und der Niederschlag abgesaugt. Nach Trocknen im Vakuum erhält man 5,7 g der Titelverbindung mit Schmp. ab 200° C (Zersetzung).

#### **2,2-Bis-[4-(4-tert.butoxycarbonyl-1-piperazinyloxy)phenyl]propan (39)**

5 g Bisphenol A-bis(chloroformat) werden in 50 ml Dichlormethan gelöst und unter Eiskühlung 7,3 ml Diisopropylethylamin und 6,6 g 1-tert.Butoxycarbonylpiperazin zugegeben. Die Mischung wird 1h bei Raumtemperatur gerührt und dann dreimal mit eiskalter 0,5 N Salzsäurelösung und zweimal mit 1 N Natronlauge extrahiert. Nach Trocknen mit Magnesiumsulfat wird am Rotationsverdampfer eingedampft und der Feststoff im Vakuum getrocknet. Man erhält 8,4 g der Titelverbindung mit Schmp. 171–172 °C.

25

#### **Beispiel 15:**

#### **Biologische Untersuchungen**

30

Die dokumentierten pathophysiologischen Effekte der Mastzell-Tryptase werden direkt durch die enzymatische Aktivität der Protease bewirkt. Dementsprechend werden sie durch Inhibitoren, die die enzymatische Aktivität der Tryptase hemmen, reduziert bzw. blockiert. Ein geeignetes Maß für die Affinität eines reversiblen Inhibitors zur Zielprotease ist die Gleichgewichts-Dissoziationskonstante  $K_i$  des Enzym-Inhibitor-Komplexes. Dieser  $K_i$ -Wert kann über den Einfluss des Inhibitors auf die Tryptase-induzierte Spaltung eines chromogenen Peptid-p-Nitroanilid-Substrates bestimmt werden.

35

**Methodik**

Die Dissoziationskonstanten für die Tryptase-Inhibitor-Komplexe werden unter Gleichgewichtsbedingungen entsprechend den allgemeinen Vorschlägen von Bieth (Bieth JG, Pathophysiological Interpretation of kinetic constants of protease inhibitors, Bull. Europ. Physiopath. Resp.

- 5 16:183-195, 1980) und den Methoden von Sommerhoff et al. (Sommerhoff CP et al., A Kazal-type inhibitor of human mast cell tryptase: Isolation from the medical leech *Hirudo medicinalis*, characterization, and sequence analysis, Biol. Chem. Hoppe-Seyler 375: 685-694, 1994) bestimmt.

- 10 Menschliche Tryptase wird aus Lungengewebe rein dargestellt; die mittels Titration bestimmte spezifische Aktivität der isolierten Protease beträgt üblicherweise 85 % des theoretischen Wertes. Konstante Mengen der Tryptase werden in Gegenwart von 50 µg/ml Heparin zur Stabilisierung der Protease mit aufsteigenden Mengen der Inhibitoren inkubiert. Nach Gleichgewichtseinstellung zwischen den Reaktionspartnern wird die verbleibende Enzymaktivität nach
- 15 Zugabe des Peptid-p-Nitroanilid-Substrates tos-Gly-Pro-Arg-pNA bestimmt, dessen Spaltung über 3 min bei 405 nm verfolgt wird. Alternativ kann die enzymatische Restaktivität auch mit fluorogenen Substraten bestimmt werden. Die apparenten Dissoziationskonstanten  $K_{iapp}$  (d.h. in der Gegenwart von Substrat) werden anschließend durch Anpassung der Enzymgeschwindigkeiten an die allgemeine Gleichung für reversible Inhibitoren (Morrison JF, Kinetics of the
- 20 reversible inhibition of enzyme-catalysed reactions by tight-binding inhibitors, Biochim. Biophys. Acta 185, 269-286, 1969) mittels nicht linearer Regression ermittelt:

$$V_i/V_0 = 1 - \{E_t + I_t + K_{iapp} - [(E_t + I_t + K_{iapp})^2 - 4E_t I_t]^{1/2}\} / 2E_t$$

- 25 Dabei sind  $V_i$  und  $V_0$  die Geschwindigkeiten in der Gegenwart bzw. Abwesenheit des Inhibitors und  $E_t$  und  $I_t$  die Konzentrationen der Tryptase und des Inhibitors.

Die für die erfindungsgemäßen Verbindungen ermittelten apparenten Dissoziationskonstanten ergeben sich aus der folgenden Tabelle A, in der die Nummern der Verbindungen den

- 30 Nummern der Verbindungen in den Beispielen entsprechen.

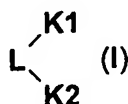
**Tabelle A**

Hemmung der humanen Tryptase

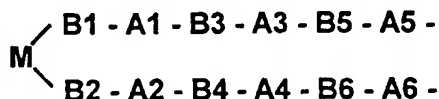
| Verbindung | K <sub>iapp</sub> (μM) |
|------------|------------------------|
| 1          | 3                      |
| 11         | 0,03                   |
| 15         | 3                      |
| 17         | 22                     |
| 21         | 0,1                    |
| 23         | 0,8                    |
| 31         | 0,2                    |
| 34         | 2                      |
| 36         | 0,028                  |

# **Patentansprüche**

1. Bifunktionelle Inhibitoren von humaner Trypsase der Formel I

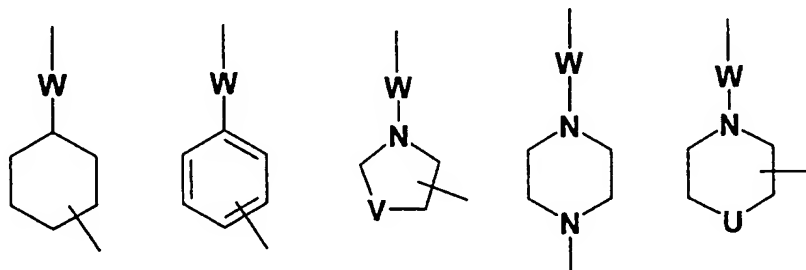


- 5 dadurch gekennzeichnet,  
dass die beiden Kopfgruppen K1 und K2 gleich oder verschieden sind und jeweils eine Gruppe Q umfassen, die mit einer Carboxylatgruppe Wechselwirkungen eingehen kann,  
der Linker L eine Konformation einnehmen kann, so daß die Gruppen Q der beiden Kopfgruppen in einem Abstand von 20 bis 45 Å vorliegen,
- 10 die Ausmaße der Kopfgruppen und des Linkers das Eindringen des Inhibitors in einen Hohlraum mit den Dimensionen 52 Å x 32 Å x 40 Å erlauben, und  
L für



steht, worin

- 15 A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,
- A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind
- 20 aus der Gruppe



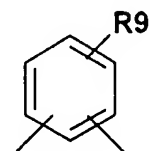
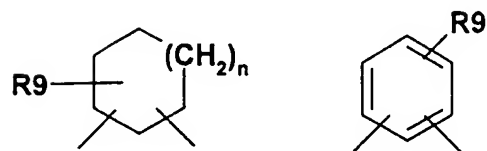
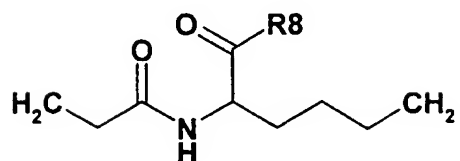
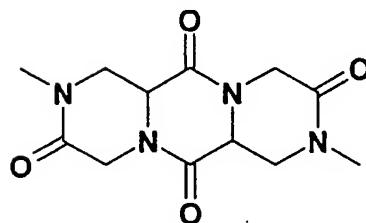
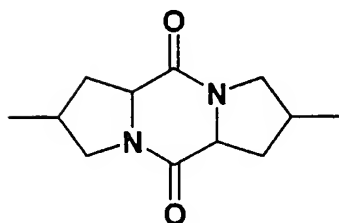
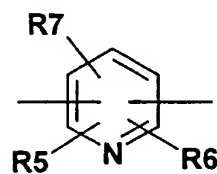
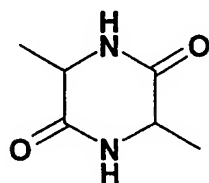
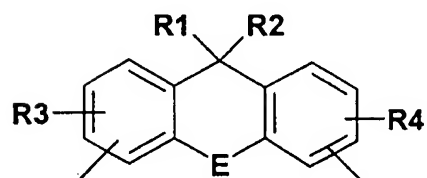
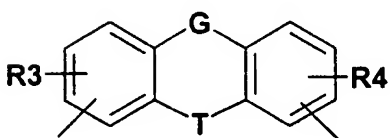
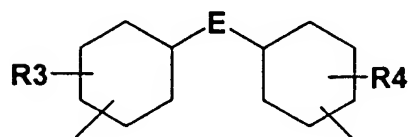
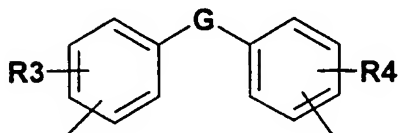
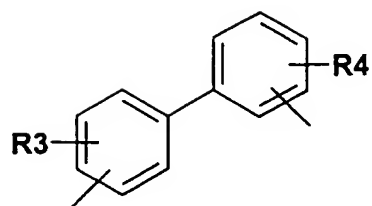
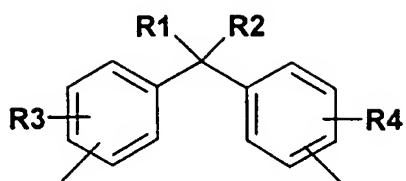
wobei

- U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),  
V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen) bedeutet, und  
W die Gruppe -C(O)- oder eine Bindung bedeutet,

A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen

-74-

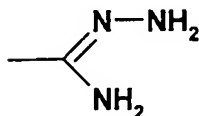
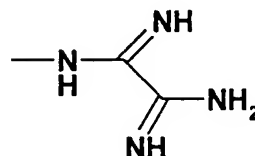
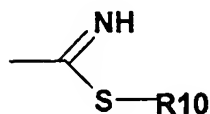
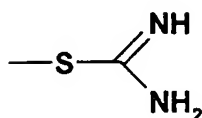
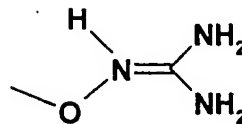
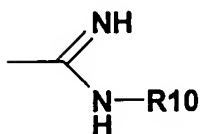
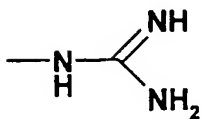
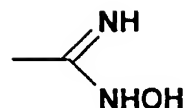
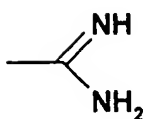
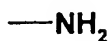


-75-

wobei

- R1 und R2 gleich oder verschieden sind und Wasserstoff, 1-4C-Alkyl, ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl oder Hydroxy bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind
- 5 -C(O)- bedeuten oder einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,
- R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,
- E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,
- 10 G -S-, -O- oder -S(O)<sub>2</sub>- bedeutet,
- I -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,
- R5 und R6 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,
- R7 Wasserstoff, 1-4C-Alkyl, Phenyl oder Pyridyl bedeutet,
- R8 1-4C-Alkoxy, N(R81)R82, Piperidino oder Morpholino bedeutet,
- 15 R81 und R82 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,
- R9 Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeutet,
- n 0, 1, 2 oder 3 bedeutet,
- K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,
- 20 K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,
- B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,
- B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,
- 25 m 0 oder 1 bedeutet,
- p 0 oder 1 bedeutet,
- X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind

-76-



wobei

R10 1-4C-Alkyl bedeutet,

Y1 und Y2 gleich oder verschieden sind und für einen 4-11C-Heteroaryl- oder 2-7C-Heterocycloalkylrest, enthaltend mindestens einen Ringstickstoff, der als Protonenakzeptor oder Protonendonator fungieren kann, stehen,

5

Z1 und Z2 gleich oder verschieden sind und 5-12C-Arylen, 5-12C-Heteroarylen, 3-8C-Cycloalkylen oder 3-8C-Heterocycloalkylen bedeuten,

wobei jedes Arylen, Heteroarylen, Cycloalkylen, Heterocycloalkylen, Heteroaryl oder Heterocycloalkyl zusätzlich seinerseits durch ein, zwei oder drei Substituenten ausgewählt aus der Gruppe Hydroxy, Halogen, Nitro, Cyano, Amino, 1-4C-Alkyl, 1-4C-Alkoxy, 1-4C-Alkoxycarbonyl, 1-4C-Alkylcarbonyloxy, Carboxyl oder Aminocarbonyl substituiert sein kann,

10

die Salze dieser Verbindungen, sowie die N-Oxide der ein Stickstoffatom enthaltenden Heteroaryle, Heterocycloalkyle, Heteroarylene und Heterocycloalkylene und deren Salze,

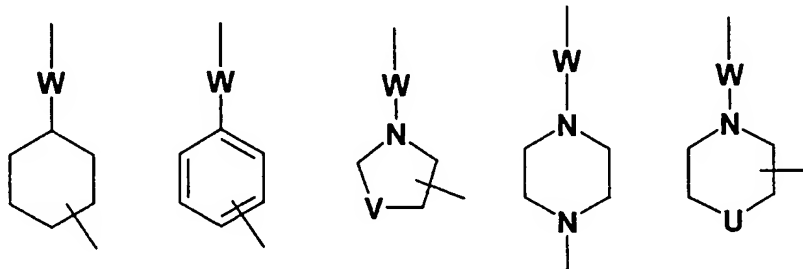
15

wobei alle diejenigen Verbindungen ausgeschlossen sind, bei denen eine oder mehrere der Variablen B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11 oder B12 die Bedeutung einer Bindung annehmen und es dadurch zur direkten Verknüpfung zweier Heteroatome, zweier Carbonylgruppen oder einer Carbonyl- und einer Thiocarbonylgruppe kommen würde.

2. Inhibitoren nach Anspruch 1, worin

A1 und A2 gleich oder verschieden sind und -C(O)-, -NH-, -O- (Sauerstoff), -S- (Schwefel), -S(O)<sub>2</sub>-, -S(O)<sub>2</sub>-NH-, -NH-S(O)<sub>2</sub>-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

5 A3 und A4 gleich oder verschieden sind und -C(O)-, -C(S)-, -O-, -S-, -NH-, -O-C(O)-, -C(O)-O-, -C(O)-NH-, -NH-C(O)- oder eine Bindung bedeuten, oder ausgewählt sind aus der Gruppe



wobei

U -O- (Sauerstoff) oder -CH<sub>2</sub>- (Methylen),

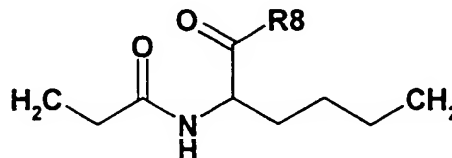
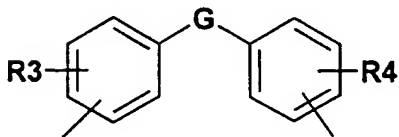
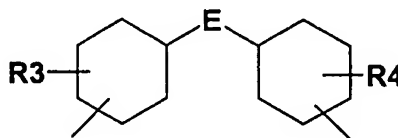
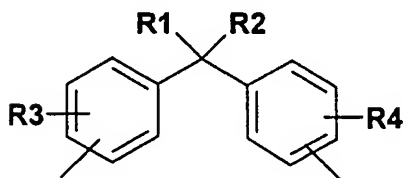
10 V -O- (Sauerstoff), -S- (Schwefel) oder -CH<sub>2</sub>- (Methylen), und

W die Gruppe -C(O)- oder eine Bindung bedeutet,

A5 und A6 gleich oder verschieden sind und -C(O)-, -NH-, -O-, -S-, -C(O)-NH-, -NH-C(O)-, -O-C(O)-, -C(O)-O- oder eine Bindung bedeuten,

M ausgewählt ist aus einer der nachfolgenden Gruppen

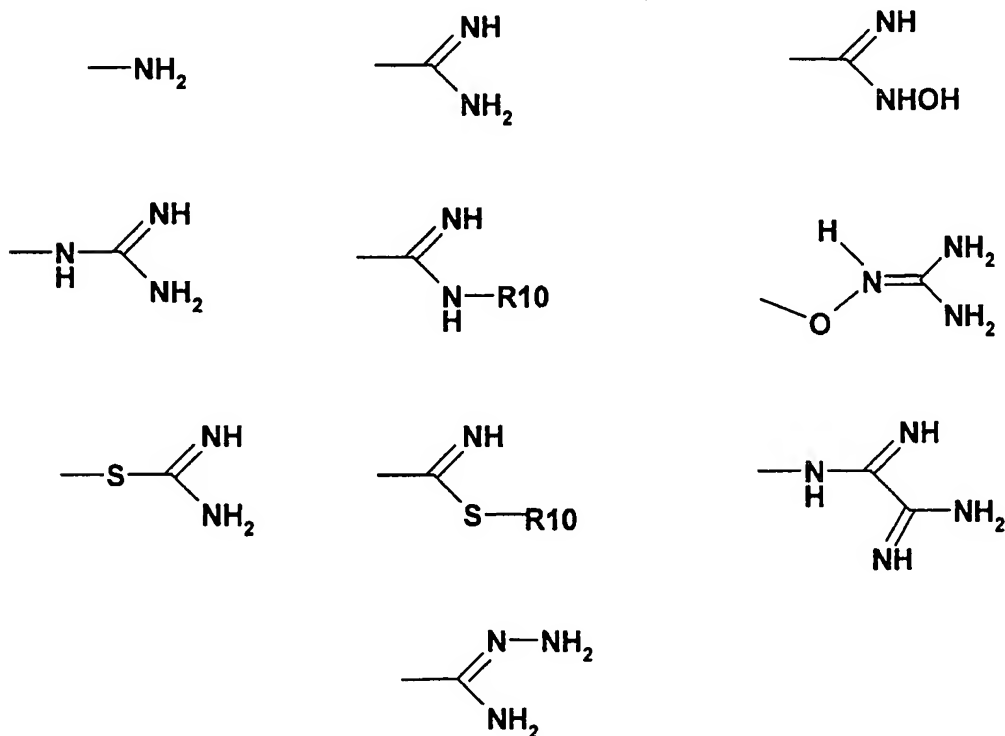
15



wobei

R1 und R2 gleich oder verschieden sind und Wasserstoff, 1-4C-Alkyl, ganz oder teilweise durch Fluor substituiertes 1-4C-Alkyl oder Hydroxy bedeuten, oder R1 und R2 gemeinsam und unter Einschluß des Kohlenstoffatoms an das sie gebunden sind  
20 -C(O)- bedeuten oder einen 5- oder 6-gliedrigen, gewünschtenfalls substituierten cyclischen Kohlenwasserstoff darstellen,

- R3 und R4 gleich oder verschieden sind und Wasserstoff oder ein, zwei oder drei gleiche oder verschiedene 1-4C-Alkylreste bedeuten,
- E -CH<sub>2</sub>-, -O- oder eine Bindung bedeutet,
- G -S-, -O- oder -S(O)<sub>2</sub>- bedeutet,
- 5 R8 1-4C-Alkoxy, N(81)R82, Piperidino oder Morpholino bedeutet,  
R81 und R82 gleich oder verschieden sind und Wasserstoff oder 1-4C-Alkyl bedeuten,
- K1 -B7-(C(O))<sub>m</sub>-B9-X1, -B7-(C(O))<sub>m</sub>-B9-Y1 oder -B7-(C(O))<sub>m</sub>-B9-Z1-B11-X1 bedeutet,
- K2 -B8-(C(O))<sub>p</sub>-B10-X2, -B8-(C(O))<sub>p</sub>-B10-Y2 oder -B8-(C(O))<sub>p</sub>-B10-Z2-B12-X2 bedeutet,  
B1, B2, B3, B4, B5 und B6 gleich oder verschieden sind und eine Bindung oder 1-4C-Alkylen bedeuten,
- 10 B7, B8, B9, B10, B11 und B12 gleich oder verschieden sind und eine Bindung oder 1-3C-Alkylen bedeuten,
- m 0 oder 1 bedeutet,
- p 0 oder 1 bedeutet,
- 15 X1 und X2 gleich oder verschieden und ausgewählt aus den nachfolgenden Gruppen sind



wobei

R10 1-4C-Alkyl bedeutet,

- Y1 und Y2 gleich oder verschieden sind und für einen 4-11C-Heteroaryl- oder 2-7C-Heterocycloalkylrest, enthaltend mindestens einen Ringstickstoff, der als Protonenakzeptor oder Protonendonator fungieren kann, stehen,
- 20

|      |     |      |     |    |         |        |        |      |       |
|------|-----|------|-----|----|---------|--------|--------|------|-------|
| ATOM | 611 | H    | GLN | 71 | -13.081 | 28.911 | 0.512  | 1.00 | 0.00  |
| ATOM | 612 | HE21 | GLN | 71 | -12.037 | 29.653 | -5.618 | 1.00 | 0.00  |
| ATOM | 613 | HE22 | GLN | 71 | -12.168 | 28.043 | -6.158 | 1.00 | 0.00  |
| ATOM | 614 | N    | HIS | 72 | -11.123 | 26.375 | -0.120 | 1.00 | 20.03 |
| ATOM | 615 | CA   | HIS | 72 | -10.071 | 25.355 | -0.044 | 1.00 | 19.17 |
| ATOM | 616 | C    | HIS | 72 | -10.131 | 24.631 | 1.290  | 1.00 | 18.35 |
| ATOM | 617 | O    | HIS | 72 | -9.950  | 25.235 | 2.338  | 1.00 | 19.70 |
| ATOM | 618 | CB   | HIS | 72 | -8.682  | 25.982 | -0.244 | 1.00 | 17.61 |
| ATOM | 619 | CG   | HIS | 72 | -8.401  | 26.399 | -1.655 | 1.00 | 15.96 |
| ATOM | 620 | ND1  | HIS | 72 | -8.205  | 25.491 | -2.671 | 1.00 | 16.94 |
| ATOM | 621 | CD2  | HIS | 72 | -8.296  | 27.623 | -2.223 | 1.00 | 16.08 |
| ATOM | 622 | CE1  | HIS | 72 | -7.995  | 26.135 | -3.806 | 1.00 | 16.70 |
| ATOM | 623 | NE2  | HIS | 72 | -8.046  | 27.431 | -3.561 | 1.00 | 16.59 |
| ATOM | 624 | H    | HIS | 72 | -11.383 | 26.777 | 0.736  | 1.00 | 0.00  |
| ATOM | 625 | HD1  | HIS | 72 | -8.222  | 24.518 | -2.533 | 1.00 | 0.00  |
| ATOM | 626 | HE2  | HIS | 72 | -7.969  | 28.083 | -4.294 | 1.00 | 0.00  |
| ATOM | 627 | N    | LEU | 73 | -10.371 | 23.330 | 1.244  | 1.00 | 17.32 |
| ATOM | 628 | CA   | LEU | 73 | -10.476 | 22.537 | 2.455  | 1.00 | 18.76 |
| ATOM | 629 | C    | LEU | 73 | -9.246  | 22.514 | 3.333  | 1.00 | 22.16 |
| ATOM | 630 | O    | LEU | 73 | -8.115  | 22.469 | 2.839  | 1.00 | 24.82 |
| ATOM | 631 | CB   | LEU | 73 | -10.806 | 21.094 | 2.110  | 1.00 | 18.94 |
| ATOM | 632 | CG   | LEU | 73 | -12.248 | 20.683 | 1.871  | 1.00 | 18.81 |
| ATOM | 633 | CD1  | LEU | 73 | -12.257 | 19.215 | 1.533  | 1.00 | 17.74 |
| ATOM | 634 | CD2  | LEU | 73 | -13.085 | 20.951 | 3.114  | 1.00 | 19.33 |
| ATOM | 635 | H    | LEU | 73 | -10.461 | 22.916 | 0.364  | 1.00 | 0.00  |
| ATOM | 636 | N    | TYR | 74 | -9.482  | 22.509 | 4.641  | 1.00 | 23.85 |
| ATOM | 637 | CA   | TYR | 74 | -8.418  | 22.410 | 5.639  | 1.00 | 26.21 |
| ATOM | 638 | C    | TYR | 74 | -7.565  | 23.648 | 5.843  | 1.00 | 28.99 |
| ATOM | 639 | O    | TYR | 74 | -6.861  | 23.764 | 6.850  | 1.00 | 28.06 |
| ATOM | 640 | CB   | TYR | 74 | -7.531  | 21.203 | 5.327  | 1.00 | 25.42 |
| ATOM | 641 | CG   | TYR | 74 | -8.310  | 19.913 | 5.213  | 1.00 | 24.73 |
| ATOM | 642 | CD1  | TYR | 74 | -8.242  | 19.127 | 4.066  | 1.00 | 24.41 |
| ATOM | 643 | CD2  | TYR | 74 | -9.117  | 19.477 | 6.259  | 1.00 | 24.55 |
| ATOM | 644 | CE1  | TYR | 74 | -8.962  | 17.931 | 3.972  | 1.00 | 24.16 |
| ATOM | 645 | CE2  | TYR | 74 | -9.835  | 18.296 | 6.172  | 1.00 | 24.01 |
| ATOM | 646 | CZ   | TYR | 74 | -9.753  | 17.529 | 5.034  | 1.00 | 23.90 |
| ATOM | 647 | OH   | TYR | 74 | -10.460 | 16.355 | 4.986  | 1.00 | 24.94 |
| ATOM | 648 | H    | TYR | 74 | -10.400 | 22.700 | 4.941  | 1.00 | 0.00  |
| ATOM | 649 | HH   | TYR | 74 | -10.745 | 16.249 | 5.896  | 1.00 | 0.00  |
| ATOM | 650 | N    | TYR | 75 | -7.616  | 24.566 | 4.888  | 1.00 | 33.29 |
| ATOM | 651 | CA   | TYR | 75 | -6.858  | 25.799 | 4.983  | 1.00 | 38.52 |
| ATOM | 652 | C    | TYR | 75 | -7.854  | 26.852 | 5.445  | 1.00 | 40.33 |
| ATOM | 653 | O    | TYR | 75 | -8.827  | 27.122 | 4.743  | 1.00 | 42.11 |
| ATOM | 654 | CB   | TYR | 75 | -6.311  | 26.172 | 3.608  | 1.00 | 43.34 |
| ATOM | 655 | CG   | TYR | 75 | -5.257  | 27.257 | 3.624  | 1.00 | 48.90 |
| ATOM | 656 | CD1  | TYR | 75 | -4.230  | 27.237 | 4.566  | 1.00 | 51.16 |
| ATOM | 657 | CD2  | TYR | 75 | -5.272  | 28.293 | 2.681  | 1.00 | 50.46 |
| ATOM | 658 | CE1  | TYR | 75 | -3.244  | 28.213 | 4.575  | 1.00 | 52.90 |
| ATOM | 659 | CE2  | TYR | 75 | -4.282  | 29.277 | 2.682  | 1.00 | 52.70 |
| ATOM | 660 | CZ   | TYR | 75 | -3.271  | 29.226 | 3.635  | 1.00 | 53.28 |
| ATOM | 661 | OH   | TYR | 75 | -2.268  | 30.166 | 3.654  | 1.00 | 55.24 |
| ATOM | 662 | H    | TYR | 75 | -8.234  | 24.493 | 4.132  | 1.00 | 0.00  |
| ATOM | 663 | HH   | TYR | 75 | -1.763  | 30.054 | 4.464  | 1.00 | 0.00  |
| ATOM | 664 | N    | GLN | 79 | -7.604  | 27.444 | 6.612  | 1.00 | 40.07 |
| ATOM | 665 | CA   | GLN | 79 | -8.487  | 28.465 | 7.190  | 1.00 | 40.38 |
| ATOM | 666 | C    | GLN | 79 | -9.684  | 27.832 | 7.920  | 1.00 | 38.64 |
| ATOM | 667 | O    | GLN | 79 | -10.735 | 28.466 | 8.081  | 1.00 | 39.81 |
| ATOM | 668 | CB   | GLN | 79 | -8.996  | 29.447 | 6.111  | 1.00 | 42.74 |
| ATOM | 669 | CG   | GLN | 79 | -7.931  | 30.318 | 5.448  | 1.00 | 46.37 |
| ATOM | 670 | CD   | GLN | 79 | -7.771  | 31.671 | 6.129  | 1.00 | 49.21 |
| ATOM | 671 | OE1  | GLN | 79 | -7.180  | 31.775 | 7.206  | 1.00 | 51.15 |
| ATOM | 672 | NE2  | GLN | 79 | -8.304  | 32.715 | 5.502  | 1.00 | 49.52 |
| ATOM | 673 | H    | GLN | 79 | -6.807  | 27.165 | 7.100  | 1.00 | 0.00  |

|      |     |         |    |         |        |        |      |       |
|------|-----|---------|----|---------|--------|--------|------|-------|
| ATOM | 674 | HE21GLN | 79 | -8.771  | 32.562 | 4.658  | 1.00 | 0.00  |
| ATOM | 675 | HE22GLN | 79 | -8.188  | 33.583 | 5.939  | 1.00 | 0.00  |
| ATOM | 676 | N ASP   | 80 | -9.510  | 26.601 | 8.390  | 1.00 | 35.73 |
| ATOM | 677 | CA ASP  | 80 | -10.571 | 25.887 | 9.100  | 1.00 | 34.10 |
| ATOM | 678 | C ASP   | 80 | -11.075 | 26.641 | 10.330 | 1.00 | 33.62 |
| ATOM | 679 | O ASP   | 80 | -10.312 | 27.332 | 11.005 | 1.00 | 33.62 |
| ATOM | 680 | CB ASP  | 80 | -10.087 | 24.498 | 9.522  | 1.00 | 33.12 |
| ATOM | 681 | CG ASP  | 80 | -10.660 | 23.377 | 8.666  | 1.00 | 30.78 |
| ATOM | 682 | OD1 ASP | 80 | -10.736 | 22.246 | 9.179  | 1.00 | 30.93 |
| ATOM | 683 | OD2 ASP | 80 | -11.025 | 23.595 | 7.496  | 1.00 | 28.71 |
| ATOM | 684 | H ASP   | 80 | -8.660  | 26.148 | 8.245  | 1.00 | 0.00  |
| ATOM | 685 | N GLN   | 81 | -12.365 | 26.495 | 10.613 | 1.00 | 33.72 |
| ATOM | 686 | CA GLN  | 81 | -13.009 | 27.145 | 11.757 | 1.00 | 33.44 |
| ATOM | 687 | C GLN   | 81 | -14.191 | 26.240 | 12.097 | 1.00 | 30.54 |
| ATOM | 688 | O GLN   | 81 | -15.320 | 26.467 | 11.658 | 1.00 | 30.41 |
| ATOM | 689 | CB GLN  | 81 | -13.483 | 28.551 | 11.357 | 1.00 | 36.68 |
| ATOM | 690 | CG GLN  | 81 | -13.389 | 29.596 | 12.474 | 1.00 | 40.37 |
| ATOM | 691 | CD GLN  | 81 | -12.982 | 30.985 | 11.971 | 1.00 | 41.54 |
| ATOM | 692 | OE1 GLN | 81 | -13.248 | 31.995 | 12.624 | 1.00 | 41.99 |
| ATOM | 693 | NE2 GLN | 81 | -12.313 | 31.033 | 10.823 | 1.00 | 41.82 |
| ATOM | 694 | H GLN   | 81 | -12.900 | 25.932 | 10.012 | 1.00 | 0.00  |
| ATOM | 695 | HE21GLN | 81 | -12.086 | 30.226 | 10.311 | 1.00 | 0.00  |
| ATOM | 696 | HE22GLN | 81 | -12.063 | 31.933 | 10.537 | 1.00 | 0.00  |
| ATOM | 697 | N LEU   | 82 | -13.905 | 25.201 | 12.871 | 1.00 | 27.16 |
| ATOM | 698 | CA LEU  | 82 | -14.889 | 24.192 | 13.238 | 1.00 | 25.21 |
| ATOM | 699 | C LEU   | 82 | -15.956 | 24.546 | 14.278 | 1.00 | 24.92 |
| ATOM | 700 | O LEU   | 82 | -15.653 | 25.043 | 15.362 | 1.00 | 25.74 |
| ATOM | 701 | CB LEU  | 82 | -14.151 | 22.910 | 13.625 | 1.00 | 24.18 |
| ATOM | 702 | CG LEU  | 82 | -13.484 | 22.068 | 12.519 | 1.00 | 23.08 |
| ATOM | 703 | CD1 LEU | 82 | -13.434 | 22.791 | 11.179 | 1.00 | 23.13 |
| ATOM | 704 | CD2 LEU | 82 | -12.093 | 21.656 | 12.956 | 1.00 | 21.60 |
| ATOM | 705 | H LEU   | 82 | -13.004 | 25.116 | 13.239 | 1.00 | 0.00  |
| ATOM | 706 | N LEU   | 83 | -17.205 | 24.239 | 13.937 | 1.00 | 23.29 |
| ATOM | 707 | CA LEU  | 83 | -18.365 | 24.504 | 14.782 | 1.00 | 23.01 |
| ATOM | 708 | C LEU   | 83 | -18.968 | 23.190 | 15.295 | 1.00 | 25.00 |
| ATOM | 709 | O LEU   | 83 | -19.281 | 22.293 | 14.505 | 1.00 | 26.30 |
| ATOM | 710 | CB LEU  | 83 | -19.430 | 25.224 | 13.958 | 1.00 | 21.83 |
| ATOM | 711 | CG LEU  | 83 | -19.050 | 26.463 | 13.154 | 1.00 | 20.51 |
| ATOM | 712 | CD1 LEU | 83 | -19.941 | 26.572 | 11.929 | 1.00 | 20.74 |
| ATOM | 713 | CD2 LEU | 83 | -19.173 | 27.691 | 14.017 | 1.00 | 20.24 |
| ATOM | 714 | H LEU   | 83 | -17.375 | 23.844 | 13.064 | 1.00 | 0.00  |
| ATOM | 715 | N PRO   | 84 | -19.155 | 23.058 | 16.621 | 1.00 | 25.46 |
| ATOM | 716 | CA PRO  | 84 | -19.727 | 21.829 | 17.182 | 1.00 | 24.91 |
| ATOM | 717 | C PRO   | 84 | -21.213 | 21.666 | 16.850 | 1.00 | 25.60 |
| ATOM | 718 | O PRO   | 84 | -21.914 | 22.643 | 16.585 | 1.00 | 25.04 |
| ATOM | 719 | CB PRO  | 84 | -19.479 | 22.000 | 18.676 | 1.00 | 24.22 |
| ATOM | 720 | CG PRO  | 84 | -19.588 | 23.482 | 18.861 | 1.00 | 24.55 |
| ATOM | 721 | CD PRO  | 84 | -18.802 | 24.007 | 17.692 | 1.00 | 25.52 |
| ATOM | 722 | N VAL   | 85 | -21.684 | 20.425 | 16.869 | 1.00 | 27.16 |
| ATOM | 723 | CA VAL  | 85 | -23.074 | 20.120 | 16.553 | 1.00 | 28.55 |
| ATOM | 724 | C VAL   | 85 | -23.908 | 19.821 | 17.793 | 1.00 | 30.63 |
| ATOM | 725 | O VAL   | 85 | -23.676 | 18.833 | 18.491 | 1.00 | 32.61 |
| ATOM | 726 | CB VAL  | 85 | -23.170 | 18.934 | 15.568 | 1.00 | 27.90 |
| ATOM | 727 | CG1 VAL | 85 | -24.607 | 18.456 | 15.435 | 1.00 | 28.88 |
| ATOM | 728 | CG2 VAL | 85 | -22.644 | 19.357 | 14.208 | 1.00 | 29.34 |
| ATOM | 729 | H VAL   | 85 | -21.105 | 19.676 | 17.121 | 1.00 | 0.00  |
| ATOM | 730 | N SER   | 86 | -24.911 | 20.660 | 18.025 | 1.00 | 30.56 |
| ATOM | 731 | CA SER  | 86 | -25.808 | 20.535 | 19.166 | 1.00 | 29.15 |
| ATOM | 732 | C SER   | 86 | -26.830 | 19.400 | 19.079 | 1.00 | 28.49 |
| ATOM | 733 | O SER   | 86 | -27.235 | 18.855 | 20.106 | 1.00 | 28.98 |
| ATOM | 734 | CB SER  | 86 | -26.535 | 21.863 | 19.379 | 1.00 | 30.43 |
| ATOM | 735 | OG SER  | 86 | -27.681 | 21.727 | 20.201 | 1.00 | 32.21 |
| ATOM | 736 | H SER   | 86 | -25.070 | 21.384 | 17.397 | 1.00 | 0.00  |

|      |     |      |     |    |         |        |        |      |       |
|------|-----|------|-----|----|---------|--------|--------|------|-------|
| ATOM | 737 | HG   | SER | 86 | -27.507 | 21.131 | 20.938 | 1.00 | 0.00  |
| ATOM | 738 | N    | ARG | 87 | -27.250 | 19.029 | 17.876 | 1.00 | 27.18 |
| ATOM | 739 | CA   | ARG | 87 | -28.255 | 17.982 | 17.764 | 1.00 | 25.82 |
| ATOM | 740 | C    | ARG | 87 | -28.304 | 17.379 | 16.378 | 1.00 | 23.86 |
| ATOM | 741 | O    | ARG | 87 | -28.177 | 18.088 | 15.385 | 1.00 | 24.82 |
| ATOM | 742 | CB   | ARG | 87 | -29.611 | 18.579 | 18.130 | 1.00 | 27.87 |
| ATOM | 743 | CG   | ARG | 87 | -30.763 | 17.612 | 18.209 | 1.00 | 31.25 |
| ATOM | 744 | CD   | ARG | 87 | -31.804 | 18.129 | 19.194 | 1.00 | 33.08 |
| ATOM | 745 | NE   | ARG | 87 | -32.101 | 19.544 | 18.986 | 1.00 | 35.62 |
| ATOM | 746 | CZ   | ARG | 87 | -33.310 | 20.035 | 18.728 | 1.00 | 37.75 |
| ATOM | 747 | NH1  | ARG | 87 | -34.358 | 19.220 | 18.645 | 1.00 | 38.48 |
| ATOM | 748 | NH2  | ARG | 87 | -33.465 | 21.344 | 18.538 | 1.00 | 38.20 |
| ATOM | 749 | H    | ARG | 87 | -26.909 | 19.486 | 17.083 | 1.00 | 0.00  |
| ATOM | 750 | HE   | ARG | 87 | -31.355 | 20.209 | 19.029 | 1.00 | 0.00  |
| ATOM | 751 | HH11 | ARG | 87 | -34.227 | 18.237 | 18.780 | 1.00 | 0.00  |
| ATOM | 752 | HH12 | ARG | 87 | -35.276 | 19.561 | 18.448 | 1.00 | 0.00  |
| ATOM | 753 | HH21 | ARG | 87 | -32.629 | 21.934 | 18.565 | 1.00 | 0.00  |
| ATOM | 754 | HH22 | ARG | 87 | -34.305 | 21.936 | 18.312 | 1.00 | 0.00  |
| ATOM | 755 | N    | ILE | 88 | -28.476 | 16.064 | 16.320 | 1.00 | 21.59 |
| ATOM | 756 | CA   | ILE | 88 | -28.544 | 15.353 | 15.052 | 1.00 | 20.21 |
| ATOM | 757 | C    | ILE | 88 | -29.915 | 14.727 | 14.929 | 1.00 | 19.59 |
| ATOM | 758 | O    | ILE | 88 | -30.256 | 13.816 | 15.677 | 1.00 | 20.48 |
| ATOM | 759 | CB   | ILE | 88 | -27.482 | 14.230 | 14.969 | 1.00 | 19.70 |
| ATOM | 760 | CG1  | ILE | 88 | -26.078 | 14.824 | 15.045 | 1.00 | 17.67 |
| ATOM | 761 | CG2  | ILE | 88 | -27.640 | 13.443 | 13.679 | 1.00 | 19.91 |
| ATOM | 762 | H    | ILE | 88 | -28.574 | 15.534 | 17.132 | 1.00 | 0.00  |
| ATOM | 763 | CD   | ILE | 88 | -25.001 | 13.807 | 14.868 | 1.00 | 17.79 |
| ATOM | 764 | N    | ILE | 89 | -30.713 | 15.223 | 14.000 | 1.00 | 19.07 |
| ATOM | 765 | CA   | ILE | 89 | -32.051 | 14.691 | 13.810 | 1.00 | 19.44 |
| ATOM | 766 | C    | ILE | 89 | -32.087 | 13.962 | 12.484 | 1.00 | 20.82 |
| ATOM | 767 | O    | ILE | 89 | -32.102 | 14.583 | 11.424 | 1.00 | 22.94 |
| ATOM | 768 | CB   | ILE | 89 | -33.095 | 15.813 | 13.807 | 1.00 | 18.56 |
| ATOM | 769 | CG1  | ILE | 89 | -33.022 | 16.594 | 15.114 | 1.00 | 17.07 |
| ATOM | 770 | CG2  | ILE | 89 | -34.479 | 15.238 | 13.613 | 1.00 | 18.47 |
| ATOM | 771 | H    | ILE | 89 | -30.385 | 15.934 | 13.407 | 1.00 | 0.00  |
| ATOM | 772 | CD   | ILE | 89 | -33.865 | 17.829 | 15.114 | 1.00 | 16.99 |
| ATOM | 773 | N    | VAL | 90 | -32.046 | 12.642 | 12.538 | 1.00 | 20.90 |
| ATOM | 774 | CA   | VAL | 90 | -32.065 | 11.843 | 11.324 | 1.00 | 21.39 |
| ATOM | 775 | C    | VAL | 90 | -33.493 | 11.364 | 11.092 | 1.00 | 22.46 |
| ATOM | 776 | O    | VAL | 90 | -34.143 | 10.891 | 12.022 | 1.00 | 24.16 |
| ATOM | 777 | CB   | VAL | 90 | -31.103 | 10.655 | 11.452 | 1.00 | 20.39 |
| ATOM | 778 | CG1  | VAL | 90 | -31.174 | 9.775  | 10.221 | 1.00 | 22.04 |
| ATOM | 779 | CG2  | VAL | 90 | -29.687 | 11.163 | 11.660 | 1.00 | 19.57 |
| ATOM | 780 | H    | VAL | 90 | -32.032 | 12.196 | 13.411 | 1.00 | 0.00  |
| ATOM | 781 | N    | HIS | 91 | -33.982 | 11.494 | 9.863  | 1.00 | 21.62 |
| ATOM | 782 | CA   | HIS | 91 | -35.342 | 11.090 | 9.546  | 1.00 | 21.27 |
| ATOM | 783 | C    | HIS | 91 | -35.671 | 9.705  | 10.080 | 1.00 | 24.29 |
| ATOM | 784 | O    | HIS | 91 | -35.018 | 8.729  | 9.728  | 1.00 | 26.00 |
| ATOM | 785 | CB   | HIS | 91 | -35.591 | 11.127 | 8.050  | 1.00 | 19.12 |
| ATOM | 786 | CG   | HIS | 91 | -37.038 | 11.055 | 7.697  | 1.00 | 18.43 |
| ATOM | 787 | ND1  | HIS | 91 | -37.848 | 12.170 | 7.659  | 1.00 | 19.05 |
| ATOM | 788 | CD2  | HIS | 91 | -37.842 | 9.999  | 7.438  | 1.00 | 18.81 |
| ATOM | 789 | CE1  | HIS | 91 | -39.089 | 11.804 | 7.396  | 1.00 | 19.27 |
| ATOM | 790 | NE2  | HIS | 91 | -39.112 | 10.491 | 7.259  | 1.00 | 20.03 |
| ATOM | 791 | H    | HIS | 91 | -33.413 | 11.823 | 9.134  | 1.00 | 0.00  |
| ATOM | 792 | HD1  | HIS | 91 | -37.556 | 13.103 | 7.789  | 1.00 | 0.00  |
| ATOM | 793 | HE2  | HIS | 91 | -39.916 | 9.963  | 7.018  | 1.00 | 0.00  |
| ATOM | 794 | N    | PRO | 92 | -36.764 | 9.595  | 10.856 | 1.00 | 25.65 |
| ATOM | 795 | CA   | PRO | 92 | -37.272 | 8.371  | 11.489 | 1.00 | 25.80 |
| ATOM | 796 | C    | PRO | 92 | -37.663 | 7.213  | 10.583 | 1.00 | 25.25 |
| ATOM | 797 | O    | PRO | 92 | -37.997 | 6.137  | 11.067 | 1.00 | 25.72 |
| ATOM | 798 | CB   | PRO | 92 | -38.480 | 8.874  | 12.280 | 1.00 | 25.50 |
| ATOM | 799 | CG   | PRO | 92 | -38.958 | 10.024 | 11.452 | 1.00 | 26.33 |

|      |     |      |     |    |         |        |        |      |       |
|------|-----|------|-----|----|---------|--------|--------|------|-------|
| ATOM | 800 | CD   | PRO | 92 | -37.667 | 10.725 | 11.138 | 1.00 | 26.34 |
| ATOM | 801 | N    | GLN | 93 | -37.607 | 7.411  | 9.275  | 1.00 | 24.91 |
| ATOM | 802 | CA   | GLN | 93 | -37.986 | 6.342  | 8.365  | 1.00 | 25.03 |
| ATOM | 803 | C    | GLN | 93 | -36.799 | 5.914  | 7.522  | 1.00 | 23.48 |
| ATOM | 804 | O    | GLN | 93 | -36.928 | 5.091  | 6.614  | 1.00 | 23.84 |
| ATOM | 805 | CB   | GLN | 93 | -39.137 | 6.797  | 7.467  | 1.00 | 27.86 |
| ATOM | 806 | CG   | GLN | 93 | -39.907 | 5.652  | 6.830  | 1.00 | 32.58 |
| ATOM | 807 | CD   | GLN | 93 | -41.337 | 5.550  | 7.334  | 1.00 | 34.52 |
| ATOM | 808 | OE1  | GLN | 93 | -42.279 | 5.524  | 6.538  | 1.00 | 35.99 |
| ATOM | 809 | NE2  | GLN | 93 | -41.508 | 5.487  | 8.650  | 1.00 | 35.14 |
| ATOM | 810 | H    | GLN | 93 | -37.226 | 8.231  | 8.932  | 1.00 | 0.00  |
| ATOM | 811 | HE21 | GLN | 93 | -40.750 | 5.500  | 9.270  | 1.00 | 0.00  |
| ATOM | 812 | HE22 | GLN | 93 | -42.422 | 5.421  | 9.002  | 1.00 | 0.00  |
| ATOM | 813 | N    | PHE | 94 | -35.635 | 6.462  | 7.845  | 1.00 | 21.31 |
| ATOM | 814 | CA   | PHE | 94 | -34.433 | 6.154  | 7.105  | 1.00 | 13.60 |
| ATOM | 815 | C    | PHE | 94 | -33.709 | 4.931  | 7.607  | 1.00 | 19.15 |
| ATOM | 816 | O    | PHE | 94 | -33.532 | 4.739  | 8.809  | 1.00 | 19.49 |
| ATOM | 817 | CB   | PHE | 94 | -33.468 | 7.343  | 7.117  | 1.00 | 16.76 |
| ATOM | 818 | CG   | PHE | 94 | -32.115 | 7.031  | 6.532  | 1.00 | 16.50 |
| ATOM | 819 | CD1  | PHE | 94 | -31.952 | 6.873  | 5.157  | 1.00 | 16.91 |
| ATOM | 820 | CD2  | PHE | 94 | -31.012 | 6.840  | 7.356  | 1.00 | 15.00 |
| ATOM | 821 | CE1  | PHE | 94 | -30.712 | 6.523  | 4.613  | 1.00 | 15.04 |
| ATOM | 822 | CE2  | PHE | 94 | -29.778 | 6.492  | 6.820  | 1.00 | 14.09 |
| ATOM | 823 | CZ   | PHE | 94 | -29.631 | 6.332  | 5.445  | 1.00 | 13.44 |
| ATOM | 824 | H    | PHE | 94 | -35.514 | 7.063  | 8.608  | 1.00 | 0.00  |
| ATOM | 825 | N    | TYR | 95 | -33.337 | 4.080  | 6.665  | 1.00 | 20.32 |
| ATOM | 826 | CA   | TYR | 95 | -32.548 | 2.903  | 6.955  | 1.00 | 20.78 |
| ATOM | 827 | C    | TYR | 95 | -31.482 | 2.744  | 5.864  | 1.00 | 22.99 |
| ATOM | 828 | O    | TYR | 95 | -30.344 | 2.374  | 6.153  | 1.00 | 23.36 |
| ATOM | 829 | CB   | TYR | 95 | -33.379 | 1.631  | 7.039  | 1.00 | 19.68 |
| ATOM | 830 | CG   | TYR | 95 | -32.487 | 0.500  | 7.478  | 1.00 | 21.06 |
| ATOM | 831 | CD1  | TYR | 95 | -31.796 | 0.585  | 8.687  | 1.00 | 22.14 |
| ATOM | 832 | CD2  | TYR | 95 | -32.232 | -0.591 | 6.652  | 1.00 | 20.20 |
| ATOM | 833 | CE1  | TYR | 95 | -30.868 | -0.371 | 9.063  | 1.00 | 20.28 |
| ATOM | 834 | CE2  | TYR | 95 | -31.296 | -1.562 | 7.022  | 1.00 | 19.85 |
| ATOM | 835 | CZ   | TYR | 95 | -30.618 | -1.434 | 8.234  | 1.00 | 19.61 |
| ATOM | 836 | OH   | TYR | 95 | -29.671 | -2.350 | 8.613  | 1.00 | 20.26 |
| ATOM | 837 | H    | TYR | 95 | -33.634 | 4.272  | 5.751  | 1.00 | 0.00  |
| ATOM | 838 | HH   | TYR | 95 | -29.220 | -2.102 | 9.428  | 1.00 | 0.00  |
| ATOM | 839 | N    | THR | 96 | -31.844 | 3.059  | 4.620  | 1.00 | 24.27 |
| ATOM | 840 | CA   | THR | 96 | -30.937 | 2.946  | 3.480  | 1.00 | 24.65 |
| ATOM | 841 | C    | THR | 96 | -31.291 | 3.982  | 2.423  | 1.00 | 24.64 |
| ATOM | 842 | O    | THR | 96 | -32.441 | 4.414  | 2.323  | 1.00 | 25.67 |
| ATOM | 843 | CB   | THR | 96 | -31.057 | 1.552  | 2.819  | 1.00 | 26.28 |
| ATOM | 844 | OG1  | THR | 96 | -30.662 | 0.534  | 3.746  | 1.00 | 29.19 |
| ATOM | 845 | CG2  | THR | 96 | -30.197 | 1.451  | 1.576  | 1.00 | 27.15 |
| ATOM | 846 | H    | THR | 96 | -32.755 | 3.375  | 4.424  | 1.00 | 0.00  |
| ATOM | 847 | HG1  | THR | 96 | -30.132 | 0.910  | 4.470  | 1.00 | 0.00  |
| ATOM | 848 | N    | ALA | 97 | -30.303 | 4.358  | 1.616  | 1.00 | 23.80 |
| ATOM | 849 | CA   | ALA | 97 | -30.509 | 5.316  | 0.537  | 1.00 | 21.68 |
| ATOM | 850 | C    | ALA | 97 | -31.517 | 4.776  | -0.473 | 1.00 | 19.74 |
| ATOM | 851 | O    | ALA | 97 | -32.474 | 5.458  | -0.799 | 1.00 | 20.20 |
| ATOM | 852 | CB   | ALA | 97 | -29.188 | 5.625  | -0.153 | 1.00 | 22.02 |
| ATOM | 853 | H    | ALA | 97 | -29.401 | 4.013  | 1.756  | 1.00 | 0.00  |
| ATOM | 854 | N    | GLN | 98 | -31.320 | 3.542  | -0.938 | 1.00 | 18.47 |
| ATOM | 855 | CA   | GLN | 98 | -32.229 | 2.937  | -1.914 | 1.00 | 18.65 |
| ATOM | 856 | C    | GLN | 98 | -33.658 | 2.880  | -1.422 | 1.00 | 13.60 |
| ATOM | 857 | O    | GLN | 98 | -34.596 | 2.993  | -2.205 | 1.00 | 18.49 |
| ATOM | 858 | CB   | GLN | 98 | -31.817 | 1.514  | -2.277 | 1.00 | 13.52 |
| ATOM | 859 | CG   | GLN | 98 | -30.435 | 1.369  | -2.838 | 1.00 | 21.00 |
| ATOM | 860 | CD   | GLN | 98 | -29.409 | 1.347  | -1.757 | 1.00 | 22.65 |
| ATOM | 861 | OE1  | GLN | 98 | -28.723 | 2.335  | -1.524 | 1.00 | 24.35 |
| ATOM | 862 | NE2  | GLN | 98 | -29.340 | 0.236  | -1.031 | 1.00 | 24.36 |

|      |     |      |     |     |         |        |        |      |       |
|------|-----|------|-----|-----|---------|--------|--------|------|-------|
| ATOM | 863 | H    | GLN | 98  | -30.515 | 3.078  | -0.638 | 1.00 | 0.00  |
| ATOM | 864 | HE21 | GLN | 98  | -29.971 | -0.487 | -1.229 | 1.00 | 0.00  |
| ATOM | 865 | HE22 | GLN | 98  | -28.636 | 0.202  | -0.349 | 1.00 | 0.00  |
| ATOM | 866 | N    | ILE | 99  | -33.821 | 2.639  | -0.130 | 1.00 | 19.53 |
| ATOM | 867 | CA   | ILE | 99  | -35.146 | 2.548  | 0.452  | 1.00 | 20.09 |
| ATOM | 868 | C    | ILE | 99  | -35.808 | 3.916  | 0.417  | 1.00 | 20.67 |
| ATOM | 869 | O    | ILE | 99  | -37.001 | 4.014  | 0.140  | 1.00 | 23.92 |
| ATOM | 870 | CB   | ILE | 99  | -35.104 | 1.989  | 1.892  | 1.00 | 20.58 |
| ATOM | 871 | CG1  | ILE | 99  | -34.840 | 0.478  | 1.881  | 1.00 | 20.42 |
| ATOM | 872 | CG2  | ILE | 99  | -36.422 | 2.226  | 2.584  | 1.00 | 22.88 |
| ATOM | 873 | H    | ILE | 99  | -33.040 | 2.561  | 0.444  | 1.00 | 0.00  |
| ATOM | 874 | CD   | ILE | 99  | -33.485 | 0.060  | 1.351  | 1.00 | 21.10 |
| ATOM | 875 | N    | GLY | 100 | -35.040 | 4.963  | 0.695  | 1.00 | 18.92 |
| ATOM | 876 | CA   | GLY | 100 | -35.588 | 6.309  | 0.657  | 1.00 | 17.35 |
| ATOM | 877 | C    | GLY | 100 | -35.422 | 7.060  | 1.960  | 1.00 | 16.46 |
| ATOM | 878 | O    | GLY | 100 | -34.850 | 6.529  | 2.911  | 1.00 | 17.40 |
| ATOM | 879 | H    | GLY | 100 | -34.118 | 4.851  | 1.002  | 1.00 | 0.00  |
| ATOM | 880 | N    | ALA | 101 | -35.909 | 8.297  | 1.993  | 1.00 | 14.63 |
| ATOM | 881 | CA   | ALA | 101 | -35.848 | 9.158  | 3.176  | 1.00 | 12.97 |
| ATOM | 882 | C    | ALA | 101 | -34.435 | 9.457  | 3.641  | 1.00 | 13.20 |
| ATOM | 883 | O    | ALA | 101 | -34.144 | 9.478  | 4.835  | 1.00 | 13.48 |
| ATOM | 884 | CB   | ALA | 101 | -36.664 | 8.569  | 4.311  | 1.00 | 12.66 |
| ATOM | 885 | H    | ALA | 101 | -36.349 | 8.638  | 1.183  | 1.00 | 0.00  |
| ATOM | 886 | N    | ASP | 102 | -33.568 | 9.745  | 2.682  | 1.00 | 14.67 |
| ATOM | 887 | CA   | ASP | 102 | -32.180 | 10.055 | 2.967  | 1.00 | 13.53 |
| ATOM | 888 | C    | ASP | 102 | -32.048 | 11.545 | 3.231  | 1.00 | 13.84 |
| ATOM | 889 | O    | ASP | 102 | -31.530 | 12.288 | 2.402  | 1.00 | 13.97 |
| ATOM | 890 | CB   | ASP | 102 | -31.312 | 9.661  | 1.775  | 1.00 | 12.12 |
| ATOM | 891 | CG   | ASP | 102 | -29.868 | 9.518  | 2.136  | 1.00 | 12.08 |
| ATOM | 892 | OD1  | ASP | 102 | -29.391 | 10.224 | 3.050  | 1.00 | 12.61 |
| ATOM | 893 | OD2  | ASP | 102 | -29.191 | 8.684  | 1.507  | 1.00 | 12.27 |
| ATOM | 894 | H    | ASP | 102 | -33.858 | 9.759  | 1.749  | 1.00 | 0.00  |
| ATOM | 895 | N    | ILE | 103 | -32.534 | 11.984 | 4.385  | 1.00 | 13.35 |
| ATOM | 896 | CA   | ILE | 103 | -32.452 | 13.390 | 4.749  | 1.00 | 12.32 |
| ATOM | 897 | C    | ILE | 103 | -32.223 | 13.469 | 6.257  | 1.00 | 12.42 |
| ATOM | 898 | O    | ILE | 103 | -32.628 | 12.564 | 6.996  | 1.00 | 11.46 |
| ATOM | 899 | CB   | ILE | 103 | -33.751 | 14.129 | 4.347  | 1.00 | 12.33 |
| ATOM | 900 | CG1  | ILE | 103 | -33.562 | 15.638 | 4.434  | 1.00 | 13.80 |
| ATOM | 901 | CG2  | ILE | 103 | -34.897 | 13.715 | 5.248  | 1.00 | 13.02 |
| ATOM | 902 | H    | ILE | 103 | -32.951 | 11.345 | 5.005  | 1.00 | 0.00  |
| ATOM | 903 | CD   | ILE | 103 | -34.742 | 16.432 | 3.908  | 1.00 | 14.33 |
| ATOM | 904 | N    | ALA | 104 | -31.518 | 14.506 | 6.705  | 1.00 | 12.64 |
| ATOM | 905 | CA   | ALA | 104 | -31.237 | 14.715 | 8.127  | 1.00 | 12.48 |
| ATOM | 906 | C    | ALA | 104 | -30.831 | 16.163 | 8.382  | 1.00 | 13.80 |
| ATOM | 907 | O    | ALA | 104 | -30.411 | 16.870 | 7.458  | 1.00 | 14.31 |
| ATOM | 908 | CB   | ALA | 104 | -30.155 | 13.775 | 8.606  | 1.00 | 13.23 |
| ATOM | 909 | H    | ALA | 104 | -31.138 | 15.162 | 6.089  | 1.00 | 0.00  |
| ATOM | 910 | N    | LEU | 105 | -30.974 | 16.598 | 9.633  | 1.00 | 14.87 |
| ATOM | 911 | CA   | LEU | 105 | -30.664 | 17.968 | 10.049 | 1.00 | 14.83 |
| ATOM | 912 | C    | LEU | 105 | -29.656 | 17.994 | 11.191 | 1.00 | 16.78 |
| ATOM | 913 | O    | LEU | 105 | -29.661 | 17.115 | 12.060 | 1.00 | 17.00 |
| ATOM | 914 | CB   | LEU | 105 | -31.936 | 18.666 | 10.532 | 1.00 | 13.18 |
| ATOM | 915 | CG   | LEU | 105 | -33.088 | 18.896 | 9.560  | 1.00 | 14.03 |
| ATOM | 916 | CD1  | LEU | 105 | -34.388 | 19.133 | 10.323 | 1.00 | 13.59 |
| ATOM | 917 | CD2  | LEU | 105 | -32.752 | 20.067 | 8.660  | 1.00 | 14.51 |
| ATOM | 918 | H    | LEU | 105 | -31.302 | 15.963 | 10.302 | 1.00 | 0.00  |
| ATOM | 919 | N    | LEU | 106 | -28.811 | 19.018 | 11.198 | 1.00 | 18.71 |
| ATOM | 920 | CA   | LEU | 106 | -27.812 | 19.188 | 12.244 | 1.00 | 20.93 |
| ATOM | 921 | C    | LEU | 106 | -27.994 | 20.582 | 12.836 | 1.00 | 24.16 |
| ATOM | 922 | O    | LEU | 106 | -27.995 | 21.581 | 12.109 | 1.00 | 23.68 |
| ATOM | 923 | CB   | LEU | 106 | -26.393 | 19.054 | 11.677 | 1.00 | 19.97 |
| ATOM | 924 | CG   | LEU | 106 | -26.056 | 17.849 | 10.790 | 1.00 | 19.78 |
| ATOM | 925 | CD1  | LEU | 106 | -24.596 | 17.905 | 10.365 | 1.00 | 19.11 |

|      |     |     |     |     |         |        |        |      |       |
|------|-----|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 926 | CD2 | LEU | 106 | -26.347 | 16.554 | 11.522 | 1.00 | 20.05 |
| ATOM | 927 | H   | LEU | 106 | -28.858 | 19.649 | 10.453 | 1.00 | 0.00  |
| ATOM | 928 | N   | GLU | 107 | -28.209 | 20.644 | 14.143 | 1.00 | 27.22 |
| ATOM | 929 | CA  | GLU | 107 | -28.375 | 21.922 | 14.815 | 1.00 | 29.48 |
| ATOM | 930 | C   | GLU | 107 | -27.040 | 22.353 | 15.405 | 1.00 | 29.97 |
| ATOM | 931 | O   | GLU | 107 | -26.405 | 21.595 | 16.141 | 1.00 | 29.53 |
| ATOM | 932 | CB  | GLU | 107 | -29.422 | 21.817 | 15.918 | 1.00 | 32.17 |
| ATOM | 933 | CG  | GLU | 107 | -29.719 | 23.143 | 16.603 | 1.00 | 35.59 |
| ATOM | 934 | CD  | GLU | 107 | -30.837 | 23.033 | 17.614 | 1.00 | 37.20 |
| ATOM | 935 | OE1 | GLU | 107 | -31.764 | 23.871 | 17.580 | 1.00 | 37.65 |
| ATOM | 936 | OE2 | GLU | 107 | -30.805 | 22.092 | 18.436 | 1.00 | 39.60 |
| ATOM | 937 | H   | GLU | 107 | -28.246 | 19.812 | 14.647 | 1.00 | 0.00  |
| ATOM | 938 | N   | LEU | 108 | -26.599 | 23.551 | 15.041 | 1.00 | 30.82 |
| ATOM | 939 | CA  | LEU | 108 | -25.343 | 24.108 | 15.523 | 1.00 | 32.08 |
| ATOM | 940 | C   | LEU | 108 | -25.564 | 24.576 | 16.948 | 1.00 | 35.24 |
| ATOM | 941 | O   | LEU | 108 | -26.621 | 25.124 | 17.256 | 1.00 | 35.84 |
| ATOM | 942 | CB  | LEU | 108 | -24.928 | 25.295 | 14.654 | 1.00 | 28.82 |
| ATOM | 943 | CG  | LEU | 108 | -24.770 | 25.020 | 13.159 | 1.00 | 25.99 |
| ATOM | 944 | CD1 | LEU | 108 | -24.518 | 26.311 | 12.411 | 1.00 | 24.24 |
| ATOM | 945 | CD2 | LEU | 108 | -23.643 | 24.043 | 12.935 | 1.00 | 24.62 |
| ATOM | 946 | H   | LEU | 108 | -27.171 | 24.076 | 14.473 | 1.00 | 0.00  |
| ATOM | 947 | N   | GLU | 109 | -24.588 | 24.347 | 17.820 | 1.00 | 39.29 |
| ATOM | 948 | CA  | GLU | 109 | -24.718 | 24.761 | 19.211 | 1.00 | 43.61 |
| ATOM | 949 | C   | GLU | 109 | -25.036 | 26.254 | 19.251 | 1.00 | 46.30 |
| ATOM | 950 | O   | GLU | 109 | -25.997 | 26.677 | 19.897 | 1.00 | 47.02 |
| ATOM | 951 | CB  | GLU | 109 | -23.442 | 24.455 | 19.999 | 1.00 | 45.61 |
| ATOM | 952 | CG  | GLU | 109 | -23.635 | 24.533 | 21.512 | 1.00 | 50.99 |
| ATOM | 953 | CD  | GLU | 109 | -22.399 | 24.137 | 22.312 | 1.00 | 53.75 |
| ATOM | 954 | OE1 | GLU | 109 | -21.729 | 23.151 | 21.932 | 1.00 | 54.12 |
| ATOM | 955 | OE2 | GLU | 109 | -22.115 | 24.802 | 23.338 | 1.00 | 55.30 |
| ATOM | 956 | H   | GLU | 109 | -23.761 | 23.921 | 17.507 | 1.00 | 0.00  |
| ATOM | 957 | N   | GLU | 110 | -24.263 | 27.035 | 18.502 | 1.00 | 48.62 |
| ATOM | 958 | CA  | GLU | 110 | -24.463 | 28.479 | 18.421 | 1.00 | 50.88 |
| ATOM | 959 | C   | GLU | 110 | -24.815 | 28.826 | 16.983 | 1.00 | 50.50 |
| ATOM | 960 | O   | GLU | 110 | -24.411 | 28.125 | 16.057 | 1.00 | 51.02 |
| ATOM | 961 | CB  | GLU | 110 | -23.182 | 29.230 | 18.786 | 1.00 | 53.80 |
| ATOM | 962 | CG  | GLU | 110 | -22.666 | 29.004 | 20.186 | 1.00 | 57.89 |
| ATOM | 963 | CD  | GLU | 110 | -21.330 | 29.685 | 20.403 | 1.00 | 60.41 |
| ATOM | 964 | OE1 | GLU | 110 | -21.301 | 30.935 | 20.447 | 1.00 | 61.67 |
| ATOM | 965 | OE2 | GLU | 110 | -20.306 | 28.975 | 20.502 | 1.00 | 62.70 |
| ATOM | 966 | H   | GLU | 110 | -23.542 | 26.648 | 17.967 | 1.00 | 0.00  |
| ATOM | 967 | N   | PRO | 111 | -25.602 | 29.893 | 16.782 | 1.00 | 49.74 |
| ATOM | 968 | CA  | PRO | 111 | -26.006 | 30.332 | 15.443 | 1.00 | 49.65 |
| ATOM | 969 | C   | PRO | 111 | -24.803 | 30.832 | 14.652 | 1.00 | 49.30 |
| ATOM | 970 | O   | PRO | 111 | -23.702 | 30.950 | 15.191 | 1.00 | 49.59 |
| ATOM | 971 | CB  | PRO | 111 | -26.972 | 31.478 | 15.742 | 1.00 | 49.68 |
| ATOM | 972 | CG  | PRO | 111 | -27.569 | 31.075 | 17.055 | 1.00 | 50.22 |
| ATOM | 973 | CD  | PRO | 111 | -26.351 | 30.625 | 17.816 | 1.00 | 50.02 |
| ATOM | 974 | N   | VAL | 112 | -25.007 | 31.115 | 13.375 | 1.00 | 48.83 |
| ATOM | 975 | CA  | VAL | 112 | -23.924 | 31.617 | 12.550 | 1.00 | 50.43 |
| ATOM | 976 | C   | VAL | 112 | -24.176 | 33.078 | 12.227 | 1.00 | 53.43 |
| ATOM | 977 | O   | VAL | 112 | -25.308 | 33.558 | 12.334 | 1.00 | 53.99 |
| ATOM | 978 | CB  | VAL | 112 | -23.770 | 30.819 | 11.229 | 1.00 | 49.15 |
| ATOM | 979 | CG1 | VAL | 112 | -23.704 | 29.341 | 11.523 | 1.00 | 48.37 |
| ATOM | 980 | CG2 | VAL | 112 | -24.897 | 31.137 | 10.250 | 1.00 | 47.56 |
| ATOM | 981 | H   | VAL | 112 | -25.887 | 30.965 | 12.979 | 1.00 | 0.00  |
| ATOM | 982 | N   | LYS | 113 | -23.110 | 33.796 | 11.890 | 1.00 | 56.42 |
| ATOM | 983 | CA  | LYS | 113 | -23.214 | 35.201 | 11.516 | 1.00 | 58.82 |
| ATOM | 984 | C   | LYS | 113 | -23.289 | 35.238 | 9.994  | 1.00 | 59.61 |
| ATOM | 985 | O   | LYS | 113 | -22.279 | 35.059 | 9.307  | 1.00 | 60.14 |
| ATOM | 986 | CB  | LYS | 113 | -22.001 | 36.000 | 12.007 | 1.00 | 60.97 |
| ATOM | 987 | CG  | LYS | 113 | -22.056 | 36.404 | 13.477 | 1.00 | 63.60 |
| ATOM | 988 | CD  | LYS | 113 | -20.848 | 37.260 | 13.851 | 1.00 | 65.56 |

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 989  | CE  | LYS | 113 | -20.963 | 37.833 | 15.263 | 1.00 | 66.59 |
| ATOM | 990  | NZ  | LYS | 113 | -19.797 | 38.700 | 15.618 | 1.00 | 66.87 |
| ATOM | 991  | H   | LYS | 113 | -22.228 | 33.376 | 11.854 | 1.00 | 0.00  |
| ATOM | 992  | HZ1 | LYS | 113 | -19.738 | 39.489 | 14.941 | 1.00 | 0.00  |
| ATOM | 993  | HZ2 | LYS | 113 | -18.929 | 38.131 | 15.567 | 1.00 | 0.00  |
| ATOM | 994  | HZ3 | LYS | 113 | -19.920 | 39.073 | 16.582 | 1.00 | 0.00  |
| ATOM | 995  | N   | VAL | 114 | -24.506 | 35.388 | 9.481  | 1.00 | 59.68 |
| ATOM | 996  | CA  | VAL | 114 | -24.743 | 35.433 | 8.044  | 1.00 | 59.43 |
| ATOM | 997  | C   | VAL | 114 | -24.134 | 36.658 | 7.384  | 1.00 | 58.88 |
| ATOM | 998  | O   | VAL | 114 | -24.019 | 37.722 | 7.996  | 1.00 | 58.87 |
| ATOM | 999  | CB  | VAL | 114 | -26.249 | 35.357 | 7.715  | 1.00 | 59.79 |
| ATOM | 1000 | CG1 | VAL | 114 | -26.795 | 33.994 | 8.108  | 1.00 | 60.14 |
| ATOM | 1001 | CG2 | VAL | 114 | -27.012 | 36.469 | 8.431  | 1.00 | 59.67 |
| ATOM | 1002 | H   | VAL | 114 | -25.254 | 35.472 | 10.102 | 1.00 | 0.00  |
| ATOM | 1003 | N   | SER | 115 | -23.769 | 36.505 | 6.119  | 1.00 | 58.84 |
| ATOM | 1004 | CA  | SER | 115 | -23.159 | 37.580 | 5.363  | 1.00 | 59.81 |
| ATOM | 1005 | C   | SER | 115 | -23.151 | 37.237 | 3.879  | 1.00 | 60.42 |
| ATOM | 1006 | O   | SER | 115 | -23.634 | 36.178 | 3.467  | 1.00 | 60.17 |
| ATOM | 1007 | CB  | SER | 115 | -21.725 | 37.808 | 5.856  | 1.00 | 60.17 |
| ATOM | 1008 | OG  | SER | 115 | -20.916 | 36.661 | 5.636  | 1.00 | 60.72 |
| ATOM | 1009 | H   | SER | 115 | -23.895 | 35.635 | 5.713  | 1.00 | 0.00  |
| ATOM | 1010 | HG  | SER | 115 | -20.360 | 36.810 | 4.886  | 1.00 | 0.00  |
| ATOM | 1011 | N   | SER | 116 | -22.572 | 38.127 | 3.084  | 1.00 | 61.27 |
| ATOM | 1012 | CA  | SER | 116 | -22.483 | 37.941 | 1.643  | 1.00 | 61.74 |
| ATOM | 1013 | C   | SER | 116 | -21.660 | 36.709 | 1.255  | 1.00 | 60.52 |
| ATOM | 1014 | O   | SER | 116 | -21.806 | 36.182 | 0.153  | 1.00 | 61.20 |
| ATOM | 1015 | CB  | SER | 116 | -21.904 | 39.205 | 0.994  | 1.00 | 63.18 |
| ATOM | 1016 | OG  | SER | 116 | -20.793 | 39.696 | 1.736  | 1.00 | 64.76 |
| ATOM | 1017 | H   | SER | 116 | -22.188 | 38.950 | 3.460  | 1.00 | 0.00  |
| ATOM | 1018 | HG  | SER | 116 | -20.630 | 40.602 | 1.428  | 1.00 | 0.00  |
| ATOM | 1019 | N   | HIS | 117 | -20.817 | 36.234 | 2.164  | 1.00 | 58.55 |
| ATOM | 1020 | CA  | HIS | 117 | -19.992 | 35.065 | 1.879  | 1.00 | 56.75 |
| ATOM | 1021 | C   | HIS | 117 | -20.518 | 33.801 | 2.526  | 1.00 | 52.95 |
| ATOM | 1022 | O   | HIS | 117 | -20.192 | 32.702 | 2.090  | 1.00 | 53.41 |
| ATOM | 1023 | CB  | HIS | 117 | -18.545 | 35.302 | 2.303  | 1.00 | 60.68 |
| ATOM | 1024 | CG  | HIS | 117 | -17.862 | 36.381 | 1.521  | 1.00 | 64.54 |
| ATOM | 1025 | ND1 | HIS | 117 | -17.221 | 36.142 | 0.325  | 1.00 | 65.45 |
| ATOM | 1026 | CD2 | HIS | 117 | -17.722 | 37.706 | 1.766  | 1.00 | 65.52 |
| ATOM | 1027 | CE1 | HIS | 117 | -16.715 | 37.273 | -0.136 | 1.00 | 66.44 |
| ATOM | 1028 | NE2 | HIS | 117 | -17.006 | 38.236 | 0.720  | 1.00 | 66.78 |
| ATOM | 1029 | H   | HIS | 117 | -20.786 | 36.628 | 3.049  | 1.00 | 0.00  |
| ATOM | 1030 | HD1 | HIS | 117 | -17.135 | 35.257 | -0.103 | 1.00 | 0.00  |
| ATOM | 1031 | HE2 | HIS | 117 | -16.760 | 39.187 | 0.638  | 1.00 | 0.00  |
| ATOM | 1032 | N   | VAL | 118 | -21.294 | 33.956 | 3.594  | 1.00 | 48.18 |
| ATOM | 1033 | CA  | VAL | 118 | -21.869 | 32.808 | 4.284  | 1.00 | 43.55 |
| ATOM | 1034 | C   | VAL | 118 | -23.293 | 33.097 | 4.725  | 1.00 | 41.05 |
| ATOM | 1035 | O   | VAL | 118 | -23.528 | 33.857 | 5.659  | 1.00 | 39.90 |
| ATOM | 1036 | CB  | VAL | 118 | -21.034 | 32.400 | 5.504  | 1.00 | 41.82 |
| ATOM | 1037 | CG1 | VAL | 118 | -21.786 | 31.391 | 6.342  | 1.00 | 41.84 |
| ATOM | 1038 | CG2 | VAL | 118 | -19.729 | 31.797 | 5.046  | 1.00 | 42.49 |
| ATOM | 1039 | H   | VAL | 118 | -21.478 | 34.827 | 3.996  | 1.00 | 0.00  |
| ATOM | 1040 | N   | HIS | 119 | -24.247 | 32.510 | 4.021  | 1.00 | 38.56 |
| ATOM | 1041 | CA  | HIS | 119 | -25.642 | 32.700 | 4.354  | 1.00 | 36.61 |
| ATOM | 1042 | C   | HIS | 119 | -26.429 | 31.512 | 3.856  | 1.00 | 35.13 |
| ATOM | 1043 | O   | HIS | 119 | -25.899 | 30.671 | 3.130  | 1.00 | 34.65 |
| ATOM | 1044 | CB  | HIS | 119 | -26.189 | 34.017 | 3.792  | 1.00 | 37.24 |
| ATOM | 1045 | CG  | HIS | 119 | -26.160 | 34.108 | 2.300  | 1.00 | 37.72 |
| ATOM | 1046 | ND1 | HIS | 119 | -25.251 | 34.891 | 1.621  | 1.00 | 38.43 |
| ATOM | 1047 | CD2 | HIS | 119 | -26.950 | 33.546 | 1.354  | 1.00 | 38.87 |
| ATOM | 1048 | CE1 | HIS | 119 | -25.482 | 34.811 | 0.323  | 1.00 | 38.41 |
| ATOM | 1049 | NE2 | HIS | 119 | -26.508 | 34.000 | 0.135  | 1.00 | 39.50 |
| ATOM | 1050 | H   | HIS | 119 | -24.025 | 31.859 | 3.317  | 1.00 | 0.00  |
| ATOM | 1051 | HD1 | HIS | 119 | -24.559 | 35.419 | 2.064  | 1.00 | 0.00  |

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1052 | HE2 | HIS | 119 | -26.901 | 33.744 | -0.728 | 1.00 | 0.00  |
| ATOM | 1053 | N   | THR | 120 | -27.702 | 31.482 | 4.221  | 1.00 | 33.01 |
| ATOM | 1054 | CA  | THR | 120 | -28.590 | 30.396 | 3.874  | 1.00 | 31.34 |
| ATOM | 1055 | C   | THR | 120 | -29.019 | 30.289 | 2.414  | 1.00 | 30.45 |
| ATOM | 1056 | O   | THR | 120 | -28.808 | 31.200 | 1.610  | 1.00 | 28.82 |
| ATOM | 1057 | CB  | THR | 120 | -29.840 | 30.434 | 4.768  | 1.00 | 31.65 |
| ATOM | 1058 | OG1 | THR | 120 | -30.483 | 31.707 | 4.637  | 1.00 | 32.89 |
| ATOM | 1059 | CG2 | THR | 120 | -29.450 | 30.238 | 6.219  | 1.00 | 30.67 |
| ATOM | 1060 | H   | THR | 120 | -28.097 | 32.227 | 4.714  | 1.00 | 0.00  |
| ATOM | 1061 | HG1 | THR | 120 | -31.359 | 31.634 | 5.047  | 1.00 | 0.00  |
| ATOM | 1062 | N   | VAL | 121 | -29.592 | 29.130 | 2.095  | 1.00 | 31.55 |
| ATOM | 1063 | CA  | VAL | 121 | -30.108 | 28.795 | 0.770  | 1.00 | 31.99 |
| ATOM | 1064 | C   | VAL | 121 | -31.629 | 28.607 | 0.892  | 1.00 | 32.94 |
| ATOM | 1065 | O   | VAL | 121 | -32.110 | 27.915 | 1.793  | 1.00 | 33.66 |
| ATOM | 1066 | CB  | VAL | 121 | -29.463 | 27.493 | 0.240  | 1.00 | 30.43 |
| ATOM | 1067 | CG1 | VAL | 121 | -29.640 | 26.364 | 1.244  | 1.00 | 29.99 |
| ATOM | 1068 | CG2 | VAL | 121 | -30.057 | 27.116 | -1.094 | 1.00 | 30.16 |
| ATOM | 1069 | H   | VAL | 121 | -29.631 | 28.456 | 2.802  | 1.00 | 0.00  |
| ATOM | 1070 | N   | THR | 122 | -32.379 | 29.228 | -0.013 | 1.00 | 32.95 |
| ATOM | 1071 | CA  | THR | 122 | -33.834 | 29.147 | 0.016  | 1.00 | 32.19 |
| ATOM | 1072 | C   | THR | 122 | -34.326 | 27.738 | -0.297 | 1.00 | 30.90 |
| ATOM | 1073 | O   | THR | 122 | -33.871 | 27.117 | -1.259 | 1.00 | 31.56 |
| ATOM | 1074 | CB  | THR | 122 | -34.479 | 30.124 | -1.012 | 1.00 | 33.41 |
| ATOM | 1075 | OG1 | THR | 122 | -33.878 | 31.423 | -0.907 | 1.00 | 34.09 |
| ATOM | 1076 | CG2 | THR | 122 | -35.966 | 30.266 | -0.745 | 1.00 | 34.09 |
| ATOM | 1077 | H   | THR | 122 | -31.960 | 29.715 | -0.748 | 1.00 | 0.00  |
| ATOM | 1078 | HG1 | THR | 122 | -32.946 | 31.364 | -1.114 | 1.00 | 0.00  |
| ATOM | 1079 | N   | LEU | 123 | -35.218 | 27.222 | 0.542  | 1.00 | 29.19 |
| ATOM | 1080 | CA  | LEU | 123 | -35.799 | 25.901 | 0.325  | 1.00 | 28.50 |
| ATOM | 1081 | C   | LEU | 123 | -36.855 | 26.112 | -0.755 | 1.00 | 29.80 |
| ATOM | 1082 | O   | LEU | 123 | -37.422 | 27.197 | -0.859 | 1.00 | 30.46 |
| ATOM | 1083 | CB  | LEU | 123 | -36.450 | 25.386 | 1.605  | 1.00 | 28.03 |
| ATOM | 1084 | CG  | LEU | 123 | -35.515 | 25.125 | 2.781  | 1.00 | 26.34 |
| ATOM | 1085 | CD1 | LEU | 123 | -36.319 | 24.727 | 4.006  | 1.00 | 25.05 |
| ATOM | 1086 | CD2 | LEU | 123 | -34.529 | 24.038 | 2.397  | 1.00 | 27.11 |
| ATOM | 1087 | H   | LEU | 123 | -35.506 | 27.754 | 1.306  | 1.00 | 0.00  |
| ATOM | 1088 | N   | PRO | 124 | -37.163 | 25.077 | -1.549 | 1.00 | 31.12 |
| ATOM | 1089 | CA  | PRO | 124 | -38.161 | 25.230 | -2.608 | 1.00 | 32.49 |
| ATOM | 1090 | C   | PRO | 124 | -39.580 | 25.127 | -2.083 | 1.00 | 35.33 |
| ATOM | 1091 | O   | PRO | 124 | -39.821 | 24.512 | -1.043 | 1.00 | 37.21 |
| ATOM | 1092 | CB  | PRO | 124 | -37.857 | 24.044 | -3.509 | 1.00 | 30.44 |
| ATOM | 1093 | CG  | PRO | 124 | -37.594 | 22.973 | -2.503 | 1.00 | 30.21 |
| ATOM | 1094 | CD  | PRO | 124 | -36.746 | 23.667 | -1.432 | 1.00 | 30.84 |
| ATOM | 1095 | N   | PRO | 125 | -40.532 | 25.796 | -2.750 | 1.00 | 36.65 |
| ATOM | 1096 | CA  | PRO | 125 | -41.934 | 25.735 | -2.322 | 1.00 | 36.82 |
| ATOM | 1097 | C   | PRO | 125 | -42.461 | 24.329 | -2.641 | 1.00 | 37.18 |
| ATOM | 1098 | O   | PRO | 125 | -42.138 | 23.762 | -3.685 | 1.00 | 36.52 |
| ATOM | 1099 | CB  | PRO | 125 | -42.600 | 26.803 | -3.187 | 1.00 | 36.99 |
| ATOM | 1100 | CG  | PRO | 125 | -41.724 | 26.858 | -4.416 | 1.00 | 37.22 |
| ATOM | 1101 | CD  | PRO | 125 | -40.347 | 26.786 | -3.824 | 1.00 | 36.60 |
| ATOM | 1102 | N   | ALA | 126 | -43.278 | 23.777 | -1.752 | 1.00 | 38.36 |
| ATOM | 1103 | CA  | ALA | 126 | -43.813 | 22.424 | -1.916 | 1.00 | 40.46 |
| ATOM | 1104 | C   | ALA | 126 | -44.421 | 22.065 | -3.279 | 1.00 | 41.72 |
| ATOM | 1105 | O   | ALA | 126 | -44.518 | 20.883 | -3.634 | 1.00 | 41.30 |
| ATOM | 1106 | CB  | ALA | 126 | -44.801 | 22.123 | -0.803 | 1.00 | 40.84 |
| ATOM | 1107 | H   | ALA | 126 | -43.510 | 24.286 | -0.952 | 1.00 | 0.00  |
| ATOM | 1108 | N   | SER | 127 | -44.835 | 23.073 | -4.034 | 1.00 | 42.97 |
| ATOM | 1109 | CA  | SER | 127 | -45.436 | 22.848 | -5.339 | 1.00 | 43.75 |
| ATOM | 1110 | C   | SER | 127 | -44.394 | 22.626 | -6.436 | 1.00 | 44.29 |
| ATOM | 1111 | O   | SER | 127 | -44.645 | 21.889 | -7.400 | 1.00 | 44.51 |
| ATOM | 1112 | CB  | SER | 127 | -46.326 | 24.034 | -5.702 | 1.00 | 44.09 |
| ATOM | 1113 | OG  | SER | 127 | -45.623 | 25.254 | -5.524 | 1.00 | 44.66 |
| ATOM | 1114 | H   | SER | 127 | -44.731 | 24.003 | -3.759 | 1.00 | 0.00  |

|      |      |     |     |     |         |        |         |      |       |
|------|------|-----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1115 | HG  | SER | 127 | -46.190 | 25.974 | -5.822  | 1.00 | 0.00  |
| ATOM | 1116 | N   | GLU | 128 | -43.221 | 23.235 | -6.266  | 1.00 | 43.79 |
| ATOM | 1117 | CA  | GLU | 128 | -42.145 | 23.137 | -7.246  | 1.00 | 42.45 |
| ATOM | 1118 | C   | GLU | 128 | -41.730 | 21.699 | -7.542  | 1.00 | 41.68 |
| ATOM | 1119 | O   | GLU | 128 | -41.532 | 20.884 | -6.629  | 1.00 | 41.78 |
| ATOM | 1120 | CB  | GLU | 128 | -40.943 | 23.966 | -6.809  | 1.00 | 42.43 |
| ATOM | 1121 | CG  | GLU | 128 | -39.861 | 24.068 | -7.864  | 1.00 | 43.95 |
| ATOM | 1122 | CD  | GLU | 128 | -40.376 | 24.577 | -9.192  | 1.00 | 44.45 |
| ATOM | 1123 | OE1 | GLU | 128 | -40.728 | 25.772 | -9.271  | 1.00 | 45.29 |
| ATOM | 1124 | OE2 | GLU | 128 | -40.427 | 23.774 | -10.152 | 1.00 | 44.56 |
| ATOM | 1125 | H   | GLU | 128 | -43.034 | 23.724 | -5.442  | 1.00 | 0.00  |
| ATOM | 1126 | N   | THR | 129 | -41.567 | 21.413 | -8.830  | 1.00 | 40.75 |
| ATOM | 1127 | CA  | THR | 129 | -41.222 | 20.078 | -9.299  | 1.00 | 40.10 |
| ATOM | 1128 | C   | THR | 129 | -39.835 | 19.903 | -9.922  | 1.00 | 38.65 |
| ATOM | 1129 | O   | THR | 129 | -39.264 | 18.808 | -9.860  | 1.00 | 40.00 |
| ATOM | 1130 | CB  | THR | 129 | -42.288 | 19.602 | -10.295 | 1.00 | 41.05 |
| ATOM | 1131 | OG1 | THR | 129 | -43.575 | 19.685 | -9.669  | 1.00 | 43.53 |
| ATOM | 1132 | CG2 | THR | 129 | -42.035 | 18.158 | -10.722 | 1.00 | 41.84 |
| ATOM | 1133 | H   | THR | 129 | -41.661 | 22.158 | -9.468  | 1.00 | 0.00  |
| ATOM | 1134 | HG1 | THR | 129 | -43.764 | 20.555 | -9.295  | 1.00 | 0.00  |
| ATOM | 1135 | N   | PHE | 130 | -39.284 | 20.974 | -10.488 | 1.00 | 35.55 |
| ATOM | 1136 | CA  | PHE | 130 | -37.970 | 20.928 | -11.135 | 1.00 | 31.51 |
| ATOM | 1137 | C   | PHE | 130 | -37.977 | 19.914 | -12.276 | 1.00 | 29.64 |
| ATOM | 1138 | O   | PHE | 130 | -37.498 | 18.787 | -12.124 | 1.00 | 28.89 |
| ATOM | 1139 | CB  | PHE | 130 | -36.866 | 20.585 | -10.125 | 1.00 | 28.53 |
| ATOM | 1140 | CG  | PHE | 130 | -36.804 | 21.523 | -8.958  | 1.00 | 25.36 |
| ATOM | 1141 | CD1 | PHE | 130 | -37.300 | 21.141 | -7.719  | 1.00 | 23.73 |
| ATOM | 1142 | CD2 | PHE | 130 | -36.266 | 22.796 | -9.102  | 1.00 | 24.25 |
| ATOM | 1143 | CE1 | PHE | 130 | -37.264 | 22.013 | -6.635  | 1.00 | 23.16 |
| ATOM | 1144 | CE2 | PHE | 130 | -36.228 | 23.673 | -8.024  | 1.00 | 23.34 |
| ATOM | 1145 | CZ  | PHE | 130 | -36.727 | 23.280 | -6.788  | 1.00 | 22.01 |
| ATOM | 1146 | H   | PHE | 130 | -39.751 | 21.841 | -10.451 | 1.00 | 0.00  |
| ATOM | 1147 | N   | PRO | 131 | -38.619 | 20.271 | -13.399 | 1.00 | 28.64 |
| ATOM | 1148 | CA  | PRO | 131 | -38.700 | 19.400 | -14.568 | 1.00 | 28.29 |
| ATOM | 1149 | C   | PRO | 131 | -37.468 | 19.602 | -15.432 | 1.00 | 28.45 |
| ATOM | 1150 | O   | PRO | 131 | -36.752 | 20.598 | -15.283 | 1.00 | 28.57 |
| ATOM | 1151 | CB  | PRO | 131 | -39.958 | 19.901 | -15.266 | 1.00 | 28.54 |
| ATOM | 1152 | CG  | PRO | 131 | -39.879 | 21.363 | -15.042 | 1.00 | 28.58 |
| ATOM | 1153 | CD  | PRO | 131 | -39.447 | 21.477 | -13.591 | 1.00 | 28.98 |
| ATOM | 1154 | N   | PRO | 132 | -37.207 | 18.668 | -16.356 | 1.00 | 29.47 |
| ATOM | 1155 | CA  | PRO | 132 | -36.042 | 18.777 | -17.237 | 1.00 | 30.72 |
| ATOM | 1156 | C   | PRO | 132 | -36.038 | 20.159 | -17.876 | 1.00 | 33.13 |
| ATOM | 1157 | O   | PRO | 132 | -37.105 | 20.695 | -18.202 | 1.00 | 34.68 |
| ATOM | 1158 | CB  | PRO | 132 | -36.311 | 17.696 | -18.281 | 1.00 | 30.49 |
| ATOM | 1159 | CG  | PRO | 132 | -37.101 | 16.677 | -17.519 | 1.00 | 29.11 |
| ATOM | 1160 | CD  | PRO | 132 | -38.053 | 17.526 | -16.740 | 1.00 | 28.78 |
| ATOM | 1161 | N   | GLY | 133 | -34.855 | 20.749 | -18.017 | 1.00 | 33.87 |
| ATOM | 1162 | CA  | GLY | 133 | -34.758 | 22.069 | -18.614 | 1.00 | 33.20 |
| ATOM | 1163 | C   | GLY | 133 | -34.338 | 23.109 | -17.596 | 1.00 | 32.95 |
| ATOM | 1164 | O   | GLY | 133 | -33.735 | 24.128 | -17.942 | 1.00 | 33.91 |
| ATOM | 1165 | H   | GLY | 133 | -34.040 | 20.311 | -17.702 | 1.00 | 0.00  |
| ATOM | 1166 | N   | MET | 134 | -34.658 | 22.858 | -16.335 | 1.00 | 32.05 |
| ATOM | 1167 | CA  | MET | 134 | -34.303 | 23.777 | -15.267 | 1.00 | 31.83 |
| ATOM | 1168 | C   | MET | 134 | -32.778 | 23.817 | -15.105 | 1.00 | 30.46 |
| ATOM | 1169 | O   | MET | 134 | -32.121 | 22.777 | -15.113 | 1.00 | 31.41 |
| ATOM | 1170 | CB  | MET | 134 | -34.952 | 23.307 | -13.969 | 1.00 | 34.34 |
| ATOM | 1171 | CG  | MET | 134 | -35.412 | 24.426 | -13.081 | 1.00 | 37.85 |
| ATOM | 1172 | SD  | MET | 134 | -36.862 | 25.212 | -13.761 | 1.00 | 42.47 |
| ATOM | 1173 | CE  | MET | 134 | -38.087 | 24.722 | -12.527 | 1.00 | 41.90 |
| ATOM | 1174 | H   | MET | 134 | -35.170 | 22.059 | -16.090 | 1.00 | 0.00  |
| ATOM | 1175 | N   | PRO | 135 | -32.185 | 25.014 | -15.028 | 1.00 | 28.25 |
| ATOM | 1176 | CA  | PRO | 135 | -30.727 | 25.070 | -14.870 | 1.00 | 27.90 |
| ATOM | 1177 | C   | PRO | 135 | -30.339 | 24.724 | -13.433 | 1.00 | 28.22 |

|      |      |     |     |     |         |        |         |      |       |
|------|------|-----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1178 | O   | PRO | 135 | -30.611 | 25.504 | -12.516 | 1.00 | 30.06 |
| ATOM | 1179 | CB  | PRO | 135 | -30.412 | 26.528 | -15.197 | 1.00 | 26.41 |
| ATOM | 1180 | CG  | PRO | 135 | -31.630 | 27.247 | -14.686 | 1.00 | 26.36 |
| ATOM | 1181 | CD  | PRO | 135 | -32.758 | 26.365 | -15.157 | 1.00 | 27.74 |
| ATOM | 1182 | N   | CYS | 136 | -29.722 | 23.564 | -13.225 | 1.00 | 26.87 |
| ATOM | 1183 | CA  | CYS | 136 | -29.337 | 23.175 | -11.867 | 1.00 | 25.46 |
| ATOM | 1184 | C   | CYS | 136 | -27.848 | 22.896 | -11.702 | 1.00 | 24.30 |
| ATOM | 1185 | O   | CYS | 136 | -27.158 | 22.568 | -12.667 | 1.00 | 23.91 |
| ATOM | 1186 | CB  | CYS | 136 | -30.160 | 21.970 | -11.398 | 1.00 | 24.62 |
| ATOM | 1187 | SG  | CYS | 136 | -31.969 | 22.212 | -11.392 | 1.00 | 22.42 |
| ATOM | 1188 | H   | CYS | 136 | -29.560 | 22.910 | -13.932 | 1.00 | 0.00  |
| ATOM | 1189 | N   | TRP | 137 | -27.367 | 23.020 | -10.465 | 1.00 | 24.11 |
| ATOM | 1190 | CA  | TRP | 137 | -25.959 | 22.805 | -10.135 | 1.00 | 24.88 |
| ATOM | 1191 | C   | TRP | 137 | -25.732 | 21.925 | -8.902  | 1.00 | 24.36 |
| ATOM | 1192 | O   | TRP | 137 | -26.593 | 21.819 | -8.021  | 1.00 | 25.47 |
| ATOM | 1193 | CB  | TRP | 137 | -25.268 | 24.147 | -9.892  | 1.00 | 26.67 |
| ATOM | 1194 | CG  | TRP | 137 | -25.157 | 25.014 | -11.098 | 1.00 | 28.41 |
| ATOM | 1195 | CD1 | TRP | 137 | -26.153 | 25.744 | -11.687 | 1.00 | 28.77 |
| ATOM | 1196 | CD2 | TRP | 137 | -23.983 | 25.241 | -11.871 | 1.00 | 27.98 |
| ATOM | 1197 | NE1 | TRP | 137 | -25.664 | 26.409 | -12.784 | 1.00 | 28.69 |
| ATOM | 1198 | CE2 | TRP | 137 | -24.333 | 26.114 | -12.921 | 1.00 | 28.37 |
| ATOM | 1199 | CE3 | TRP | 137 | -22.664 | 24.791 | -11.781 | 1.00 | 29.44 |
| ATOM | 1200 | CZ2 | TRP | 137 | -23.414 | 26.543 | -13.872 | 1.00 | 30.36 |
| ATOM | 1201 | CZ3 | TRP | 137 | -21.747 | 25.218 | -12.726 | 1.00 | 31.02 |
| ATOM | 1202 | CH2 | TRP | 137 | -22.125 | 26.083 | -13.759 | 1.00 | 31.41 |
| ATOM | 1203 | H   | TRP | 137 | -27.990 | 23.232 | -9.747  | 1.00 | 0.00  |
| ATOM | 1204 | HE1 | TRP | 137 | -26.175 | 27.059 | -13.299 | 1.00 | 0.00  |
| ATOM | 1205 | N   | VAL | 138 | -24.570 | 21.284 | -8.857  | 1.00 | 22.15 |
| ATOM | 1206 | CA  | VAL | 138 | -24.190 | 20.442 | -7.734  | 1.00 | 21.72 |
| ATOM | 1207 | C   | VAL | 138 | -22.841 | 20.969 | -7.286  | 1.00 | 22.73 |
| ATOM | 1208 | O   | VAL | 138 | -21.997 | 21.302 | -8.123  | 1.00 | 24.43 |
| ATOM | 1209 | CB  | VAL | 138 | -23.976 | 18.984 | -8.135  | 1.00 | 20.93 |
| ATOM | 1210 | CG1 | VAL | 138 | -23.820 | 18.135 | -6.890  | 1.00 | 21.73 |
| ATOM | 1211 | CG2 | VAL | 138 | -25.117 | 18.496 | -8.964  | 1.00 | 21.44 |
| ATOM | 1212 | H   | VAL | 138 | -23.970 | 21.370 | -9.627  | 1.00 | 0.00  |
| ATOM | 1213 | N   | THR | 139 | -22.624 | 21.021 | -5.979  | 1.00 | 20.79 |
| ATOM | 1214 | CA  | THR | 139 | -21.370 | 21.520 | -5.443  | 1.00 | 18.68 |
| ATOM | 1215 | C   | THR | 139 | -20.831 | 20.619 | -4.343  | 1.00 | 19.87 |
| ATOM | 1216 | O   | THR | 139 | -21.602 | 20.052 | -3.562  | 1.00 | 20.93 |
| ATOM | 1217 | CB  | THR | 139 | -21.555 | 22.929 | -4.889  | 1.00 | 16.45 |
| ATOM | 1218 | OG1 | THR | 139 | -22.812 | 23.005 | -4.211  | 1.00 | 16.50 |
| ATOM | 1219 | CG2 | THR | 139 | -21.548 | 23.930 | -6.005  | 1.00 | 14.04 |
| ATOM | 1220 | H   | THR | 139 | -23.333 | 20.742 | -5.369  | 1.00 | 0.00  |
| ATOM | 1221 | HG1 | THR | 139 | -23.024 | 22.161 | -3.784  | 1.00 | 0.00  |
| ATOM | 1222 | N   | GLY | 140 | -19.510 | 20.503 | -4.274  | 1.00 | 19.46 |
| ATOM | 1223 | CA  | GLY | 140 | -18.907 | 19.664 | -3.256  | 1.00 | 18.62 |
| ATOM | 1224 | C   | GLY | 140 | -17.411 | 19.506 | -3.399  | 1.00 | 17.41 |
| ATOM | 1225 | O   | GLY | 140 | -16.805 | 20.038 | -4.330  | 1.00 | 17.38 |
| ATOM | 1226 | H   | GLY | 140 | -18.948 | 20.961 | -4.940  | 1.00 | 0.00  |
| ATOM | 1227 | N   | TRP | 141 | -16.822 | 18.781 | -2.453  | 1.00 | 17.33 |
| ATOM | 1228 | CA  | TRP | 141 | -15.385 | 18.519 | -2.423  | 1.00 | 17.65 |
| ATOM | 1229 | C   | TRP | 141 | -15.154 | 17.022 | -2.583  | 1.00 | 17.27 |
| ATOM | 1230 | O   | TRP | 141 | -14.281 | 16.454 | -1.918  | 1.00 | 17.41 |
| ATOM | 1231 | CB  | TRP | 141 | -14.794 | 18.933 | -1.073  | 1.00 | 18.30 |
| ATOM | 1232 | CG  | TRP | 141 | -14.732 | 20.396 | -0.805  | 1.00 | 18.20 |
| ATOM | 1233 | CD1 | TRP | 141 | -13.745 | 21.255 | -1.184  | 1.00 | 18.41 |
| ATOM | 1234 | CD2 | TRP | 141 | -15.653 | 21.161 | -0.027  | 1.00 | 17.70 |
| ATOM | 1235 | NE1 | TRP | 141 | -13.989 | 22.504 | -0.683  | 1.00 | 18.56 |
| ATOM | 1236 | CE2 | TRP | 141 | -15.156 | 22.477 | 0.032   | 1.00 | 18.28 |
| ATOM | 1237 | CE3 | TRP | 141 | -16.851 | 20.859 | 0.633   | 1.00 | 18.76 |
| ATOM | 1238 | CZ2 | TRP | 141 | -15.813 | 23.495 | 0.724   | 1.00 | 19.77 |
| ATOM | 1239 | CZ3 | TRP | 141 | -17.506 | 21.872 | 1.323   | 1.00 | 19.19 |
| ATOM | 1240 | CH2 | TRP | 141 | -16.986 | 23.173 | 1.362   | 1.00 | 20.82 |

|      |      |      |     |     |         |        |         |      |       |
|------|------|------|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1241 | H    | TRP | 141 | -17.406 | 18.366 | -1.792  | 1.00 | 0.00  |
| ATOM | 1242 | HE1  | TRP | 141 | -13.414 | 23.289 | -0.817  | 1.00 | 0.00  |
| ATOM | 1243 | N    | GLY | 142 | -15.965 | 16.377 | -3.413  | 1.00 | 16.46 |
| ATOM | 1244 | CA   | GLY | 142 | -15.834 | 14.947 | -3.602  | 1.00 | 16.92 |
| ATOM | 1245 | C    | GLY | 142 | -14.931 | 14.507 | -4.735  | 1.00 | 17.67 |
| ATOM | 1246 | O    | GLY | 142 | -14.312 | 15.329 | -5.412  | 1.00 | 18.99 |
| ATOM | 1247 | H    | GLY | 142 | -16.690 | 16.821 | -3.903  | 1.00 | 0.00  |
| ATOM | 1248 | N    | ASP | 143 | -14.857 | 13.195 | -4.928  | 1.00 | 16.94 |
| ATOM | 1249 | CA   | ASP | 143 | -14.047 | 12.598 | -5.970  | 1.00 | 17.99 |
| ATOM | 1250 | C    | ASP | 143 | -14.314 | 13.256 | -7.307  | 1.00 | 20.06 |
| ATOM | 1251 | O    | ASP | 143 | -15.459 | 13.409 | -7.722  | 1.00 | 20.61 |
| ATOM | 1252 | CB   | ASP | 143 | -14.328 | 11.100 | -6.062  | 1.00 | 17.04 |
| ATOM | 1253 | CG   | ASP | 143 | -13.772 | 10.331 | -4.886  | 1.00 | 15.16 |
| ATOM | 1254 | OD1  | ASP | 143 | -13.263 | 10.965 | -3.937  | 1.00 | 14.81 |
| ATOM | 1255 | OD2  | ASP | 143 | -13.833 | 9.084  | -4.917  | 1.00 | 13.79 |
| ATOM | 1256 | H    | ASP | 143 | -15.356 | 12.605 | -4.335  | 1.00 | 0.00  |
| ATOM | 1257 | N    | VAL | 144 | -13.246 | 13.640 | -7.986  | 1.00 | 23.01 |
| ATOM | 1258 | CA   | VAL | 144 | -13.374 | 14.293 | -9.278  | 1.00 | 26.09 |
| ATOM | 1259 | C    | VAL | 144 | -13.688 | 13.281 | -10.366 | 1.00 | 28.14 |
| ATOM | 1260 | O    | VAL | 144 | -13.979 | 13.652 | -11.506 | 1.00 | 29.65 |
| ATOM | 1261 | CB   | VAL | 144 | -12.106 | 15.080 | -9.642  | 1.00 | 26.19 |
| ATOM | 1262 | CG1  | VAL | 144 | -11.901 | 16.200 | -8.641  | 1.00 | 25.96 |
| ATOM | 1263 | CG2  | VAL | 144 | -10.892 | 14.155 | -9.671  | 1.00 | 26.43 |
| ATOM | 1264 | H    | VAL | 144 | -12.389 | 13.374 | -7.594  | 1.00 | 0.00  |
| ATOM | 1265 | N    | ASP | 145 | -13.623 | 12.005 | -10.003 | 1.00 | 29.52 |
| ATOM | 1266 | CA   | ASP | 145 | -13.917 | 10.920 | -10.922 | 1.00 | 31.28 |
| ATOM | 1267 | C    | ASP | 145 | -14.024 | 9.638  | -10.113 | 1.00 | 31.83 |
| ATOM | 1268 | O    | ASP | 145 | -13.555 | 9.565  | -8.977  | 1.00 | 30.05 |
| ATOM | 1269 | CB   | ASP | 145 | -12.818 | 10.779 | -11.975 | 1.00 | 33.12 |
| ATOM | 1270 | CG   | ASP | 145 | -13.321 | 10.159 | -13.272 | 1.00 | 34.76 |
| ATOM | 1271 | OD1  | ASP | 145 | -13.019 | 10.718 | -14.350 | 1.00 | 35.56 |
| ATOM | 1272 | OD2  | ASP | 145 | -14.016 | 9.121  | -13.224 | 1.00 | 34.67 |
| ATOM | 1273 | H    | ASP | 145 | -13.376 | 11.754 | -9.086  | 1.00 | 0.00  |
| ATOM | 1274 | N    | ASN | 146 | -14.688 | 8.652  | -10.696 | 1.00 | 34.26 |
| ATOM | 1275 | CA   | ASN | 146 | -14.895 | 7.351  | -10.087 | 1.00 | 36.45 |
| ATOM | 1276 | C    | ASN | 146 | -13.584 | 6.916  | -9.453  | 1.00 | 37.80 |
| ATOM | 1277 | O    | ASN | 146 | -12.611 | 6.649  | -10.156 | 1.00 | 37.96 |
| ATOM | 1278 | CB   | ASN | 146 | -15.302 | 6.364  | -11.178 | 1.00 | 37.99 |
| ATOM | 1279 | CG   | ASN | 146 | -16.382 | 5.423  | -10.731 | 1.00 | 39.85 |
| ATOM | 1280 | OD1  | ASN | 146 | -17.567 | 5.654  | -10.981 | 1.00 | 40.60 |
| ATOM | 1281 | ND2  | ASN | 146 | -15.989 | 4.350  | -10.061 | 1.00 | 42.11 |
| ATOM | 1282 | H    | ASN | 146 | -15.009 | 8.813  | -11.605 | 1.00 | 0.00  |
| ATOM | 1283 | HD21 | ASN | 146 | -15.025 | 4.217  | -9.898  | 1.00 | 0.00  |
| ATOM | 1284 | HD22 | ASN | 146 | -16.668 | 3.730  | -9.734  | 1.00 | 0.00  |
| ATOM | 1285 | N    | ASP | 147 | -13.550 | 6.903  | -8.125  | 1.00 | 40.45 |
| ATOM | 1286 | CA   | ASP | 147 | -12.353 | 6.529  | -7.375  | 1.00 | 43.92 |
| ATOM | 1287 | C    | ASP | 147 | -11.154 | 7.393  | -7.758  | 1.00 | 44.87 |
| ATOM | 1288 | O    | ASP | 147 | -10.160 | 6.909  | -8.302  | 1.00 | 45.36 |
| ATOM | 1289 | CB   | ASP | 147 | -12.026 | 5.039  | -7.534  | 1.00 | 46.32 |
| ATOM | 1290 | CG   | ASP | 147 | -12.826 | 4.156  | -6.584  | 1.00 | 49.75 |
| ATOM | 1291 | OD1  | ASP | 147 | -13.227 | 4.637  | -5.495  | 1.00 | 50.63 |
| ATOM | 1292 | OD2  | ASP | 147 | -13.058 | 2.973  | -6.933  | 1.00 | 50.18 |
| ATOM | 1293 | H    | ASP | 147 | -14.314 | 7.201  | -7.591  | 1.00 | 0.00  |
| ATOM | 1294 | N    | GLU | 149 | -11.273 | 8.684  | -7.471  | 1.00 | 44.87 |
| ATOM | 1295 | CA   | GLU | 149 | -10.231 | 9.656  | -7.749  | 1.00 | 44.17 |
| ATOM | 1296 | C    | GLU | 149 | -10.398 | 10.804 | -6.764  | 1.00 | 41.75 |
| ATOM | 1297 | O    | GLU | 149 | -11.291 | 11.640 | -6.911  | 1.00 | 41.69 |
| ATOM | 1298 | CB   | GLU | 149 | -10.337 | 10.161 | -9.190  | 1.00 | 48.13 |
| ATOM | 1299 | CG   | GLU | 149 | -9.525  | 9.366  | -10.203 | 1.00 | 54.18 |
| ATOM | 1300 | CD   | GLU | 149 | -8.027  | 9.634  | -10.100 | 1.00 | 58.78 |
| ATOM | 1301 | OE1  | GLU | 149 | -7.289  | 8.776  | -9.557  | 1.00 | 60.56 |
| ATOM | 1302 | OE2  | GLU | 149 | -7.587  | 10.712 | -10.566 | 1.00 | 61.37 |
| ATOM | 1303 | H    | GLU | 149 | -12.107 | 8.995  | -7.047  | 1.00 | 0.00  |

|      |      |      |     |      |         |        |        |      |       |
|------|------|------|-----|------|---------|--------|--------|------|-------|
| ATOM | 1304 | N    | ARG | 150  | -9.537  | 10.832 | -5.756 | 1.00 | 39.44 |
| ATOM | 1305 | CA   | ARG | 150  | -9.584  | 11.863 | -4.728 | 1.00 | 38.81 |
| ATOM | 1306 | C    | ARG | 150  | -9.419  | 13.271 | -5.288 | 1.00 | 35.43 |
| ATOM | 1307 | O    | ARG | 150  | -8.768  | 13.469 | -6.309 | 1.00 | 34.38 |
| ATOM | 1308 | CB   | ARG | 150  | -8.488  | 11.614 | -3.683 | 1.00 | 42.97 |
| ATOM | 1309 | CG   | ARG | 150  | -7.062  | 11.882 | -4.183 | 1.00 | 48.22 |
| ATOM | 1310 | CD   | ARG | 150  | -6.002  | 11.501 | -3.145 | 1.00 | 51.86 |
| ATOM | 1311 | NE   | ARG | 150  | -5.315  | 12.662 | -2.581 | 1.00 | 54.43 |
| ATOM | 1312 | CZ   | ARG | 150  | -3.990  | 12.820 | -2.563 | 1.00 | 56.69 |
| ATOM | 1313 | NH1  | ARG | 150  | -3.184  | 11.894 | -3.077 | 1.00 | 56.01 |
| ATOM | 1314 | NH2  | ARG | 150  | -3.461  | 13.913 | -2.025 | 1.00 | 58.24 |
| ATOM | 1315 | H    | ARG | 150  | -8.851  | 10.139 | -5.749 | 1.00 | 0.00  |
| ATOM | 1316 | HE   | ARG | 150  | -5.913  | 13.347 | -2.204 | 1.00 | 0.00  |
| ATOM | 1317 | HH11 | ARG | 150  | -3.528  | 11.050 | -3.487 | 1.00 | 0.00  |
| ATOM | 1318 | HH12 | ARG | 150  | -2.195  | 12.061 | -3.059 | 1.00 | 0.00  |
| ATOM | 1319 | HH21 | ARG | 150  | -4.015  | 14.635 | -1.614 | 1.00 | 0.00  |
| ATOM | 1320 | HH22 | ARG | 150  | -2.459  | 14.000 | -2.054 | 1.00 | 0.00  |
| ATOM | 1321 | N    | LEU | 151  | -10.043 | 14.240 | -4.634 | 1.00 | 33.17 |
| ATOM | 1322 | CA   | LEU | 151  | -9.918  | 15.632 | -5.045 | 1.00 | 32.33 |
| ATOM | 1323 | C    | LEU | 151  | -8.483  | 16.015 | -4.669 | 1.00 | 32.56 |
| ATOM | 1324 | O    | LEU | 151  | -8.120  | 15.992 | -3.489 | 1.00 | 34.95 |
| ATOM | 1325 | CB   | LEU | 151  | -10.927 | 16.496 | -4.276 | 1.00 | 31.19 |
| ATOM | 1326 | CG   | LEU | 151  | -10.906 | 18.023 | -4.425 | 1.00 | 29.95 |
| ATOM | 1327 | CD1  | LEU | 151  | -11.280 | 18.446 | -5.840 | 1.00 | 28.73 |
| ATOM | 1328 | CD2  | LEU | 151  | -11.869 | 18.632 | -3.420 | 1.00 | 29.52 |
| ATOM | 1329 | H    | LEU | 151  | -10.610 | 14.016 | -3.869 | 1.00 | 0.00  |
| ATOM | 1330 | N    | PRO | 152  | -7.633  | 16.326 | -5.666 | 1.00 | 30.14 |
| ATOM | 1331 | CA   | PRO | 152  | -6.240  | 16.696 | -5.401 | 1.00 | 27.60 |
| ATOM | 1332 | C    | PRO | 152  | -6.087  | 17.992 | -4.601 | 1.00 | 25.89 |
| ATOM | 1333 | O    | PRO | 152  | -6.860  | 18.947 | -4.777 | 1.00 | 25.84 |
| ATOM | 1334 | CB   | PRO | 152  | -5.670  | 16.874 | -6.809 | 1.00 | 26.42 |
| ATOM | 1335 | CG   | PRO | 152  | -6.542  | 16.036 | -7.657 | 1.00 | 26.55 |
| ATOM | 1336 | CD   | PRO | 152  | -7.893  | 16.358 | -7.112 | 1.00 | 28.51 |
| ATOM | 1337 | N    | PRO | 152A | -5.127  | 18.021 | -3.659 | 1.00 | 23.33 |
| ATOM | 1338 | CA   | PRO | 152A | -4.934  | 19.244 | -2.881 | 1.00 | 21.00 |
| ATOM | 1339 | C    | PRO | 152A | -4.515  | 20.332 | -3.867 | 1.00 | 20.45 |
| ATOM | 1340 | O    | PRO | 152A | -3.860  | 20.040 | -4.868 | 1.00 | 19.44 |
| ATOM | 1341 | CB   | PRO | 152A | -3.804  | 18.863 | -1.923 | 1.00 | 19.97 |
| ATOM | 1342 | CG   | PRO | 152A | -3.098  | 17.747 | -2.616 | 1.00 | 20.16 |
| ATOM | 1343 | CD   | PRO | 152A | -4.215  | 16.959 | -3.203 | 1.00 | 22.00 |
| ATOM | 1344 | N    | PRO | 152B | -4.935  | 21.588 | -3.638 | 1.00 | 21.24 |
| ATOM | 1345 | CA   | PRO | 152B | -5.386  | 22.202 | -2.386 | 1.00 | 20.91 |
| ATOM | 1346 | C    | PRO | 152B | -6.885  | 22.091 | -2.118 | 1.00 | 20.62 |
| ATOM | 1347 | O    | PRO | 152B | -7.484  | 23.014 | -1.569 | 1.00 | 22.33 |
| ATOM | 1348 | CB   | PRO | 152B | -4.982  | 23.656 | -2.577 | 1.00 | 21.15 |
| ATOM | 1349 | CG   | PRO | 152B | -5.313  | 23.873 | -4.012 | 1.00 | 21.38 |
| ATOM | 1350 | CD   | PRO | 152B | -4.761  | 22.620 | -4.681 | 1.00 | 21.72 |
| ATOM | 1351 | N    | PHE | 153  | -7.504  | 21.017 | -2.591 | 1.00 | 19.80 |
| ATOM | 1352 | CA   | PHE | 153  | -8.929  | 20.763 | -2.366 | 1.00 | 18.06 |
| ATOM | 1353 | C    | PHE | 153  | -9.862  | 21.931 | -2.676 | 1.00 | 18.64 |
| ATOM | 1354 | O    | PHE | 153  | -10.518 | 22.481 | -1.781 | 1.00 | 18.67 |
| ATOM | 1355 | CB   | PHE | 153  | -9.151  | 20.271 | -0.935 | 1.00 | 13.82 |
| ATOM | 1356 | CG   | PHE | 153  | -8.138  | 19.263 | -0.492 | 1.00 | 10.65 |
| ATOM | 1357 | CD1  | PHE | 153  | -7.329  | 19.511 | 0.613  | 1.00 | 9.56  |
| ATOM | 1358 | CD2  | PHE | 153  | -7.950  | 18.093 | -1.214 | 1.00 | 8.00  |
| ATOM | 1359 | CE1  | PHE | 153  | -6.347  | 18.615 | 0.984  | 1.00 | 8.00  |
| ATOM | 1360 | CE2  | PHE | 153  | -6.974  | 17.198 | -0.848 | 1.00 | 8.00  |
| ATOM | 1361 | CZ   | PHE | 153  | -6.169  | 17.457 | 0.251  | 1.00 | 8.00  |
| ATOM | 1362 | H    | PHE | 153  | -7.061  | 20.371 | -3.172 | 1.00 | 0.00  |
| ATOM | 1363 | N    | PRO | 154  | -9.868  | 22.375 | -3.941 | 1.00 | 18.99 |
| ATOM | 1364 | CA   | PRO | 154  | -10.730 | 23.482 | -4.357 | 1.00 | 19.22 |
| ATOM | 1365 | C    | PRO | 154  | -12.177 | 23.004 | -4.372 | 1.00 | 20.58 |
| ATOM | 1366 | O    | PRO | 154  | -12.429 | 21.815 | -4.578 | 1.00 | 22.09 |

|      |      |      |     |     |         |        |         |      |       |
|------|------|------|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1367 | CB   | PRO | 154 | -10.245 | 23.759 | -5.774  | 1.00 | 18.84 |
| ATOM | 1368 | CG   | PRO | 154 | -9.812  | 22.409 | -6.253  | 1.00 | 18.04 |
| ATOM | 1369 | CD   | PRO | 154 | -9.041  | 21.904 | -5.068  | 1.00 | 17.93 |
| ATOM | 1370 | N    | LEU | 155 | -13.124 | 23.904 | -4.123  | 1.00 | 20.02 |
| ATOM | 1371 | CA   | LEU | 155 | -14.531 | 23.521 | -4.153  | 1.00 | 18.98 |
| ATOM | 1372 | C    | LEU | 155 | -14.952 | 23.507 | -5.617  | 1.00 | 19.90 |
| ATOM | 1373 | O    | LEU | 155 | -14.746 | 24.491 | -6.335  | 1.00 | 20.15 |
| ATOM | 1374 | CB   | LEU | 155 | -15.394 | 24.512 | -3.382  | 1.00 | 17.09 |
| ATOM | 1375 | CG   | LEU | 155 | -16.892 | 24.277 | -3.545  | 1.00 | 15.73 |
| ATOM | 1376 | CD1  | LEU | 155 | -17.267 | 23.006 | -2.838  | 1.00 | 18.10 |
| ATOM | 1377 | CD2  | LEU | 155 | -17.673 | 25.437 | -2.980  | 1.00 | 15.76 |
| ATOM | 1378 | H    | LEU | 155 | -12.909 | 24.851 | -3.954  | 1.00 | 0.00  |
| ATOM | 1379 | N    | LYS | 156 | -15.521 | 22.393 | -6.062  | 1.00 | 19.19 |
| ATOM | 1380 | CA   | LYS | 156 | -15.956 | 22.265 | -7.439  | 1.00 | 17.77 |
| ATOM | 1381 | C    | LYS | 156 | -17.478 | 22.340 | -7.546  | 1.00 | 17.11 |
| ATOM | 1382 | O    | LYS | 156 | -18.196 | 22.030 | -6.591  | 1.00 | 17.35 |
| ATOM | 1383 | CB   | LYS | 156 | -15.437 | 20.959 | -8.046  | 1.00 | 18.12 |
| ATOM | 1384 | CG   | LYS | 156 | -13.916 | 20.881 | -8.223  | 1.00 | 17.75 |
| ATOM | 1385 | CD   | LYS | 156 | -13.487 | 19.540 | -8.845  | 1.00 | 18.50 |
| ATOM | 1386 | CE   | LYS | 156 | -13.955 | 19.380 | -10.306 | 1.00 | 20.12 |
| ATOM | 1387 | NZ   | LYS | 156 | -13.777 | 17.997 | -10.879 | 1.00 | 20.18 |
| ATOM | 1388 | H    | LYS | 156 | -15.710 | 21.637 | -5.466  | 1.00 | 0.00  |
| ATOM | 1389 | HZ1  | LYS | 156 | -14.430 | 17.357 | -10.351 | 1.00 | 0.00  |
| ATOM | 1390 | HZ2  | LYS | 156 | -12.810 | 17.663 | -10.711 | 1.00 | 0.00  |
| ATOM | 1391 | HZ3  | LYS | 156 | -14.013 | 17.920 | -11.880 | 1.00 | 0.00  |
| ATOM | 1392 | N    | GLN | 157 | -17.942 | 22.829 | -8.693  | 1.00 | 15.66 |
| ATOM | 1393 | CA   | GLN | 157 | -19.358 | 22.974 | -9.013  | 1.00 | 13.71 |
| ATOM | 1394 | C    | GLN | 157 | -19.509 | 22.298 | -10.361 | 1.00 | 13.57 |
| ATOM | 1395 | O    | GLN | 157 | -18.511 | 22.068 | -11.039 | 1.00 | 13.93 |
| ATOM | 1396 | CB   | GLN | 157 | -19.717 | 24.448 | -9.193  | 1.00 | 13.33 |
| ATOM | 1397 | CG   | GLN | 157 | -19.008 | 25.099 | -10.365 | 1.00 | 14.13 |
| ATOM | 1398 | CD   | GLN | 157 | -19.338 | 26.568 | -10.525 | 1.00 | 15.78 |
| ATOM | 1399 | OE1  | GLN | 157 | -19.604 | 27.268 | -9.550  | 1.00 | 16.19 |
| ATOM | 1400 | NE2  | GLN | 157 | -19.295 | 27.052 | -11.760 | 1.00 | 16.77 |
| ATOM | 1401 | H    | GLN | 157 | -17.300 | 23.134 | -9.359  | 1.00 | 0.00  |
| ATOM | 1402 | HE21 | GLN | 157 | -19.018 | 26.439 | -12.486 | 1.00 | 0.00  |
| ATOM | 1403 | HE22 | GLN | 157 | -19.515 | 27.979 | -11.932 | 1.00 | 0.00  |
| ATOM | 1404 | N    | VAL | 158 | -20.741 | 21.997 | -10.755 | 1.00 | 14.27 |
| ATOM | 1405 | CA   | VAL | 158 | -21.011 | 21.356 | -12.041 | 1.00 | 15.15 |
| ATOM | 1406 | C    | VAL | 158 | -22.488 | 21.486 | -12.365 | 1.00 | 17.08 |
| ATOM | 1407 | O    | VAL | 158 | -23.325 | 21.388 | -11.473 | 1.00 | 20.23 |
| ATOM | 1408 | CB   | VAL | 158 | -20.620 | 19.859 | -12.034 | 1.00 | 14.74 |
| ATOM | 1409 | CG1  | VAL | 158 | -21.555 | 19.054 | -11.142 | 1.00 | 16.38 |
| ATOM | 1410 | CG2  | VAL | 158 | -20.618 | 19.312 | -13.439 | 1.00 | 15.18 |
| ATOM | 1411 | H    | VAL | 158 | -21.483 | 22.139 | -10.127 | 1.00 | 0.00  |
| ATOM | 1412 | N    | LYS | 159 | -22.806 | 21.758 | -13.624 | 1.00 | 18.36 |
| ATOM | 1413 | CA   | LYS | 159 | -24.195 | 21.908 | -14.053 | 1.00 | 19.23 |
| ATOM | 1414 | C    | LYS | 159 | -24.746 | 20.552 | -14.512 | 1.00 | 18.92 |
| ATOM | 1415 | O    | LYS | 159 | -24.273 | 19.967 | -15.490 | 1.00 | 18.64 |
| ATOM | 1416 | CB   | LYS | 159 | -24.269 | 22.927 | -15.189 | 1.00 | 20.90 |
| ATOM | 1417 | CG   | LYS | 159 | -25.671 | 23.312 | -15.630 | 1.00 | 22.93 |
| ATOM | 1418 | CD   | LYS | 159 | -25.628 | 23.843 | -17.054 | 1.00 | 24.18 |
| ATOM | 1419 | CE   | LYS | 159 | -26.881 | 24.579 | -17.421 | 1.00 | 25.27 |
| ATOM | 1420 | NZ   | LYS | 159 | -27.011 | 25.792 | -16.570 | 1.00 | 28.52 |
| ATOM | 1421 | H    | LYS | 159 | -22.093 | 21.839 | -14.285 | 1.00 | 0.00  |
| ATOM | 1422 | HZ1  | LYS | 159 | -26.160 | 26.371 | -16.715 | 1.00 | 0.00  |
| ATOM | 1423 | HZ2  | LYS | 159 | -27.095 | 25.522 | -15.568 | 1.00 | 0.00  |
| ATOM | 1424 | HZ3  | LYS | 159 | -27.840 | 26.323 | -16.909 | 1.00 | 0.00  |
| ATOM | 1425 | N    | VAL | 160 | -25.769 | 20.070 | -13.827 | 1.00 | 18.97 |
| ATOM | 1426 | CA   | VAL | 160 | -26.351 | 18.782 | -14.163 | 1.00 | 19.55 |
| ATOM | 1427 | C    | VAL | 160 | -27.766 | 18.883 | -14.716 | 1.00 | 20.23 |
| ATOM | 1428 | O    | VAL | 160 | -28.546 | 19.739 | -14.300 | 1.00 | 21.70 |
| ATOM | 1429 | CB   | VAL | 160 | -26.384 | 17.864 | -12.926 | 1.00 | 19.41 |

|      |      |         |     |     |         |        |         |      |       |
|------|------|---------|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1430 | CG1     | VAL | 160 | -24.972 | 17.540 | -12.481 | 1.00 | 19.83 |
| ATOM | 1431 | CG2     | VAL | 160 | -27.164 | 18.534 | -11.794 | 1.00 | 19.22 |
| ATOM | 1432 | H       | VAL | 160 | -26.171 | 20.632 | -13.130 | 1.00 | 0.00  |
| ATOM | 1433 | N       | PRO | 161 | -28.081 | 18.077 | -15.741 | 1.00 | 19.90 |
| ATOM | 1434 | CA      | PRO | 161 | -29.436 | 18.145 | -16.283 | 1.00 | 19.73 |
| ATOM | 1435 | C       | PRO | 161 | -30.372 | 17.284 | -15.432 | 1.00 | 19.71 |
| ATOM | 1436 | O       | PRO | 161 | -30.018 | 16.172 | -15.037 | 1.00 | 18.49 |
| ATOM | 1437 | CB      | PRO | 161 | -29.259 | 17.583 | -17.691 | 1.00 | 18.89 |
| ATOM | 1438 | CG      | PRO | 161 | -28.171 | 16.589 | -17.521 | 1.00 | 19.76 |
| ATOM | 1439 | CD      | PRO | 161 | -27.190 | 17.338 | -16.648 | 1.00 | 21.05 |
| ATOM | 1440 | N       | ILE | 162 | -31.525 | 17.849 | -15.089 | 1.00 | 20.70 |
| ATOM | 1441 | CA      | ILE | 162 | -32.548 | 17.180 | -14.293 | 1.00 | 20.87 |
| ATOM | 1442 | C       | ILE | 162 | -33.297 | 16.202 | -15.190 | 1.00 | 22.73 |
| ATOM | 1443 | O       | ILE | 162 | -33.305 | 16.364 | -16.413 | 1.00 | 23.43 |
| ATOM | 1444 | CB      | ILE | 162 | -33.575 | 18.208 | -13.779 | 1.00 | 18.92 |
| ATOM | 1445 | CG1     | ILE | 162 | -32.881 | 19.307 | -12.982 | 1.00 | 18.56 |
| ATOM | 1446 | CG2     | ILE | 162 | -34.612 | 17.538 | -12.927 | 1.00 | 19.42 |
| ATOM | 1447 | H       | ILE | 162 | -31.709 | 18.761 | -15.372 | 1.00 | 0.00  |
| ATOM | 1448 | CD      | ILE | 162 | -32.289 | 18.836 | -11.694 | 1.00 | 20.32 |
| ATOM | 1449 | N       | MET | 163 | -33.891 | 15.169 | -14.608 | 1.00 | 24.74 |
| ATOM | 1450 | CA      | MET | 163 | -34.671 | 14.239 | -15.407 | 1.00 | 28.15 |
| ATOM | 1451 | C       | MET | 163 | -35.870 | 13.631 | -14.685 | 1.00 | 28.93 |
| ATOM | 1452 | O       | MET | 163 | -35.850 | 13.423 | -13.474 | 1.00 | 30.57 |
| ATOM | 1453 | CB      | MET | 163 | -33.794 | 13.166 | -16.045 | 1.00 | 30.47 |
| ATOM | 1454 | CG      | MET | 163 | -33.211 | 12.144 | -15.114 | 1.00 | 34.74 |
| ATOM | 1455 | SD      | MET | 163 | -32.320 | 10.949 | -16.108 | 1.00 | 37.70 |
| ATOM | 1456 | CE      | MET | 163 | -31.014 | 12.027 | -16.815 | 1.00 | 37.47 |
| ATOM | 1457 | H       | MET | 163 | -33.781 | 15.028 | -13.647 | 1.00 | 0.00  |
| ATOM | 1458 | N       | GLU | 164 | -36.945 | 13.433 | -15.436 | 1.00 | 29.40 |
| ATOM | 1459 | CA      | GLU | 164 | -38.174 | 12.867 | -14.916 | 1.00 | 31.77 |
| ATOM | 1460 | C       | GLU | 164 | -37.888 | 11.586 | -14.174 | 1.00 | 31.92 |
| ATOM | 1461 | O       | GLU | 164 | -37.086 | 10.779 | -14.630 | 1.00 | 33.29 |
| ATOM | 1462 | CB      | GLU | 164 | -39.119 | 12.558 | -16.071 | 1.00 | 35.74 |
| ATOM | 1463 | CG      | GLU | 164 | -40.002 | 13.708 | -16.490 | 1.00 | 41.14 |
| ATOM | 1464 | CD      | GLU | 164 | -41.448 | 13.479 | -16.112 | 1.00 | 45.91 |
| ATOM | 1465 | OE1     | GLU | 164 | -42.319 | 14.218 | -16.620 | 1.00 | 47.97 |
| ATOM | 1466 | OE2     | GLU | 164 | -41.723 | 12.545 | -15.316 | 1.00 | 49.13 |
| ATOM | 1467 | H       | GLU | 164 | -36.916 | 13.682 | -16.380 | 1.00 | 0.00  |
| ATOM | 1468 | N       | ASN | 165 | -38.564 | 11.384 | -13.049 | 1.00 | 31.65 |
| ATOM | 1469 | CA      | ASN | 165 | -38.392 | 10.171 | -12.254 | 1.00 | 30.80 |
| ATOM | 1470 | C       | ASN | 165 | -38.757 | 8.927  | -13.054 | 1.00 | 31.68 |
| ATOM | 1471 | O       | ASN | 165 | -38.050 | 7.929  | -13.002 | 1.00 | 31.61 |
| ATOM | 1472 | CB      | ASN | 165 | -39.263 | 10.205 | -10.998 | 1.00 | 30.02 |
| ATOM | 1473 | CG      | ASN | 165 | -38.612 | 10.934 | -9.857  | 1.00 | 29.18 |
| ATOM | 1474 | OD1     | ASN | 165 | -38.243 | 12.105 | -9.976  | 1.00 | 31.19 |
| ATOM | 1475 | ND2     | ASN | 165 | -38.479 | 10.256 | -8.731  | 1.00 | 28.13 |
| ATOM | 1476 | H       | ASN | 165 | -39.169 | 12.091 | -12.754 | 1.00 | 0.00  |
| ATOM | 1477 | HD21ASN |     | 165 | -38.797 | 9.326  | -8.662  | 1.00 | 0.00  |
| ATOM | 1478 | HD22ASN |     | 165 | -38.061 | 10.716 | -7.977  | 1.00 | 0.00  |
| ATOM | 1479 | N       | HIS | 166 | -39.842 | 8.997  | -13.823 | 1.00 | 32.91 |
| ATOM | 1480 | CA      | HIS | 166 | -40.296 | 7.850  | -14.612 | 1.00 | 34.53 |
| ATOM | 1481 | C       | HIS | 166 | -39.276 | 7.405  | -15.648 | 1.00 | 32.37 |
| ATOM | 1482 | O       | HIS | 166 | -39.080 | 6.208  | -15.852 | 1.00 | 32.20 |
| ATOM | 1483 | CB      | HIS | 166 | -41.630 | 8.162  | -15.280 | 1.00 | 40.62 |
| ATOM | 1484 | CG      | HIS | 166 | -42.625 | 8.769  | -14.347 | 1.00 | 48.92 |
| ATOM | 1485 | ND1     | HIS | 166 | -42.881 | 10.125 | -14.310 | 1.00 | 51.74 |
| ATOM | 1486 | CD2     | HIS | 166 | -43.367 | 8.220  | -13.355 | 1.00 | 51.33 |
| ATOM | 1487 | CE1     | HIS | 166 | -43.732 | 10.386 | -13.334 | 1.00 | 53.49 |
| ATOM | 1488 | NE2     | HIS | 166 | -44.043 | 9.246  | -12.738 | 1.00 | 53.76 |
| ATOM | 1489 | H       | HIS | 166 | -40.297 | 9.862  | -13.892 | 1.00 | 0.00  |
| ATOM | 1490 | HD1     | HIS | 166 | -42.530 | 10.857 | -14.880 | 1.00 | 0.00  |
| ATOM | 1491 | HE2     | HIS | 166 | -44.652 | 9.158  | -11.974 | 1.00 | 0.00  |
| ATOM | 1492 | N       | ILE | 167 | -38.599 | 8.369  | -16.267 | 1.00 | 29.15 |

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|      |      |     |     |     |         |        |         |      |       |
|------|------|-----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1493 | CA  | ILE | 167 | -37.590 | 8.069  | -17.279 | 1.00 | 25.40 |
| ATOM | 1494 | C   | ILE | 167 | -36.327 | 7.595  | -16.566 | 1.00 | 24.71 |
| ATOM | 1495 | O   | ILE | 167 | -35.659 | 6.660  | -17.007 | 1.00 | 25.68 |
| ATOM | 1496 | CB  | ILE | 167 | -37.249 | 9.307  | -18.127 | 1.00 | 22.75 |
| ATOM | 1497 | CG1 | ILE | 167 | -38.530 | 10.019 | -18.592 | 1.00 | 22.09 |
| ATOM | 1498 | CG2 | ILE | 167 | -36.351 | 8.910  | -19.281 | 1.00 | 20.92 |
| ATOM | 1499 | H   | ILE | 167 | -38.744 | 9.302  | -16.017 | 1.00 | 0.00  |
| ATOM | 1500 | CD  | ILE | 167 | -39.611 | 9.109  | -19.169 | 1.00 | 21.21 |
| ATOM | 1501 | N   | CYS | 168 | -36.023 | 8.242  | -15.449 | 1.00 | 22.77 |
| ATOM | 1502 | CA  | CYS | 168 | -34.864 | 7.904  | -14.644 | 1.00 | 20.38 |
| ATOM | 1503 | C   | CYS | 168 | -34.952 | 6.467  | -14.149 | 1.00 | 13.88 |
| ATOM | 1504 | O   | CYS | 168 | -33.960 | 5.737  | -14.151 | 1.00 | 18.67 |
| ATOM | 1505 | CB  | CYS | 168 | -34.762 | 8.858  | -13.466 | 1.00 | 19.86 |
| ATOM | 1506 | SG  | CYS | 168 | -33.267 | 8.581  | -12.486 | 1.00 | 25.34 |
| ATOM | 1507 | H   | CYS | 168 | -36.547 | 9.012  | -15.155 | 1.00 | 0.00  |
| ATOM | 1508 | N   | ASP | 169 | -36.153 | 6.062  | -13.744 | 1.00 | 17.91 |
| ATOM | 1509 | CA  | ASP | 169 | -36.395 | 4.708  | -13.263 | 1.00 | 17.44 |
| ATOM | 1510 | C   | ASP | 169 | -36.147 | 3.737  | -14.408 | 1.00 | 17.43 |
| ATOM | 1511 | O   | ASP | 169 | -35.489 | 2.712  | -14.237 | 1.00 | 18.43 |
| ATOM | 1512 | CB  | ASP | 169 | -37.839 | 4.571  | -12.768 | 1.00 | 18.17 |
| ATOM | 1513 | CG  | ASP | 169 | -38.093 | 3.253  | -12.073 | 1.00 | 18.12 |
| ATOM | 1514 | OD1 | ASP | 169 | -37.473 | 2.996  | -11.030 | 1.00 | 18.81 |
| ATOM | 1515 | OD2 | ASP | 169 | -38.925 | 2.468  | -12.559 | 1.00 | 18.25 |
| ATOM | 1516 | H   | ASP | 169 | -36.893 | 6.687  | -13.710 | 1.00 | 0.00  |
| ATOM | 1517 | N   | ALA | 170 | -36.655 | 4.080  | -15.586 | 1.00 | 16.11 |
| ATOM | 1518 | CA  | ALA | 170 | -36.477 | 3.246  | -16.763 | 1.00 | 14.86 |
| ATOM | 1519 | C   | ALA | 170 | -34.997 | 3.079  | -17.069 | 1.00 | 15.28 |
| ATOM | 1520 | O   | ALA | 170 | -34.512 | 1.962  | -17.185 | 1.00 | 15.95 |
| ATOM | 1521 | CB  | ALA | 170 | -37.191 | 3.854  | -17.940 | 1.00 | 15.63 |
| ATOM | 1522 | H   | ALA | 170 | -37.200 | 4.889  | -15.640 | 1.00 | 0.00  |
| ATOM | 1523 | N   | LYS | 171 | -34.277 | 4.193  | -17.170 | 1.00 | 16.33 |
| ATOM | 1524 | CA  | LYS | 171 | -32.846 | 4.155  | -17.445 | 1.00 | 16.55 |
| ATOM | 1525 | C   | LYS | 171 | -32.196 | 3.172  | -16.493 | 1.00 | 16.60 |
| ATOM | 1526 | O   | LYS | 171 | -31.487 | 2.258  | -16.918 | 1.00 | 16.71 |
| ATOM | 1527 | CB  | LYS | 171 | -32.214 | 5.535  | -17.264 | 1.00 | 17.79 |
| ATOM | 1528 | CG  | LYS | 171 | -32.353 | 6.453  | -18.463 | 1.00 | 20.18 |
| ATOM | 1529 | CD  | LYS | 171 | -31.370 | 7.615  | -18.380 | 1.00 | 22.70 |
| ATOM | 1530 | CE  | LYS | 171 | -31.228 | 8.323  | -19.715 | 1.00 | 25.58 |
| ATOM | 1531 | NZ  | LYS | 171 | -30.907 | 7.374  | -20.840 | 1.00 | 27.76 |
| ATOM | 1532 | H   | LYS | 171 | -34.737 | 5.041  | -17.056 | 1.00 | 0.00  |
| ATOM | 1533 | HZ1 | LYS | 171 | -31.735 | 6.769  | -20.992 | 1.00 | 0.00  |
| ATOM | 1534 | HZ2 | LYS | 171 | -30.119 | 6.728  | -20.589 | 1.00 | 0.00  |
| ATOM | 1535 | HZ3 | LYS | 171 | -30.690 | 7.898  | -21.716 | 1.00 | 0.00  |
| ATOM | 1536 | N   | TYR | 172 | -32.508 | 3.325  | -15.210 | 1.00 | 16.89 |
| ATOM | 1537 | CA  | TYR | 172 | -31.977 | 2.453  | -14.168 | 1.00 | 17.35 |
| ATOM | 1538 | C   | TYR | 172 | -32.252 | 0.956  | -14.382 | 1.00 | 16.66 |
| ATOM | 1539 | O   | TYR | 172 | -31.430 | 0.121  | -14.014 | 1.00 | 16.33 |
| ATOM | 1540 | CB  | TYR | 172 | -32.478 | 2.905  | -12.791 | 1.00 | 16.98 |
| ATOM | 1541 | CG  | TYR | 172 | -31.436 | 3.666  | -12.009 | 1.00 | 16.83 |
| ATOM | 1542 | CD1 | TYR | 172 | -31.255 | 5.036  | -12.192 | 1.00 | 17.77 |
| ATOM | 1543 | CD2 | TYR | 172 | -30.595 | 3.006  | -11.123 | 1.00 | 15.99 |
| ATOM | 1544 | CE1 | TYR | 172 | -30.257 | 5.726  | -11.519 | 1.00 | 16.71 |
| ATOM | 1545 | CE2 | TYR | 172 | -29.601 | 3.679  | -10.449 | 1.00 | 16.10 |
| ATOM | 1546 | CZ  | TYR | 172 | -29.434 | 5.036  | -10.648 | 1.00 | 17.10 |
| ATOM | 1547 | OH  | TYR | 172 | -28.434 | 5.678  | -9.968  | 1.00 | 18.38 |
| ATOM | 1548 | H   | TYR | 172 | -33.092 | 4.066  | -14.938 | 1.00 | 0.00  |
| ATOM | 1549 | HH  | TYR | 172 | -28.017 | 5.006  | -9.422  | 1.00 | 0.00  |
| ATOM | 1550 | N   | HIS | 173 | -33.390 | 0.620  | -14.982 | 1.00 | 15.28 |
| ATOM | 1551 | CA  | HIS | 173 | -33.723 | -0.777 | -15.242 | 1.00 | 13.36 |
| ATOM | 1552 | C   | HIS | 173 | -32.921 | -1.375 | -16.388 | 1.00 | 14.24 |
| ATOM | 1553 | O   | HIS | 173 | -32.788 | -2.593 | -16.481 | 1.00 | 15.44 |
| ATOM | 1554 | CB  | HIS | 173 | -35.208 | -0.937 | -15.525 | 1.00 | 11.58 |
| ATOM | 1555 | CG  | HIS | 173 | -36.059 | -0.855 | -14.304 | 1.00 | 10.16 |

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|      |      |     |     |      |         |         |         |      |       |
|------|------|-----|-----|------|---------|---------|---------|------|-------|
| ATOM | 1556 | ND1 | HIS | 173  | -36.406 | -1.963  | -13.566 | 1.00 | 10.90 |
| ATOM | 1557 | CD2 | HIS | 173  | -36.606 | 0.207   | -13.666 | 1.00 | 10.92 |
| ATOM | 1558 | CE1 | HIS | 173  | -37.131 | -1.590  | -12.528 | 1.00 | 11.19 |
| ATOM | 1559 | NE2 | HIS | 173  | -37.266 | -0.278  | -12.566 | 1.00 | 11.38 |
| ATOM | 1560 | H   | HIS | 173  | -33.993 | 1.355   | -15.228 | 1.00 | 0.00  |
| ATOM | 1561 | HD1 | HIS | 173  | -36.186 | -2.896  | -13.801 | 1.00 | 0.00  |
| ATOM | 1562 | HE2 | HIS | 173  | -37.752 | 0.270   | -11.916 | 1.00 | 0.00  |
| ATOM | 1563 | N   | LEU | 173A | -32.397 | -0.532  | -17.271 | 1.00 | 14.95 |
| ATOM | 1564 | CA  | LEU | 173A | -31.604 | -1.020  | -18.396 | 1.00 | 16.44 |
| ATOM | 1565 | C   | LEU | 173A | -30.347 | -1.717  | -17.866 | 1.00 | 18.23 |
| ATOM | 1566 | O   | LEU | 173A | -29.611 | -1.161  | -17.044 | 1.00 | 18.66 |
| ATOM | 1567 | CB  | LEU | 173A | -31.206 | 0.131   | -19.321 | 1.00 | 16.19 |
| ATOM | 1568 | CG  | LEU | 173A | -32.336 | 0.973   | -19.910 | 1.00 | 15.99 |
| ATOM | 1569 | CD1 | LEU | 173A | -31.738 | 2.212   | -20.537 | 1.00 | 17.46 |
| ATOM | 1570 | CD2 | LEU | 173A | -33.149 | 0.180   | -20.925 | 1.00 | 14.77 |
| ATOM | 1571 | H   | LEU | 173A | -32.529 | 0.430   | -17.142 | 1.00 | 0.00  |
| ATOM | 1572 | N   | GLY | 173B | -30.103 | -2.931  | -19.346 | 1.00 | 19.99 |
| ATOM | 1573 | CA  | GLY | 173B | -28.946 | -3.691  | -17.903 | 1.00 | 19.63 |
| ATOM | 1574 | C   | GLY | 173B | -29.175 | -4.322  | -16.542 | 1.00 | 20.10 |
| ATOM | 1575 | O   | GLY | 173B | -28.279 | -4.966  | -16.003 | 1.00 | 19.40 |
| ATOM | 1576 | H   | GLY | 173B | -30.711 | -3.312  | -19.002 | 1.00 | 0.00  |
| ATOM | 1577 | N   | ALA | 173C | -30.380 | -4.165  | -16.006 | 1.00 | 20.43 |
| ATOM | 1578 | CA  | ALA | 173C | -30.718 | -4.708  | -14.706 | 1.00 | 21.00 |
| ATOM | 1579 | C   | ALA | 173C | -31.678 | -5.869  | -14.803 | 1.00 | 22.51 |
| ATOM | 1580 | O   | ALA | 173C | -32.476 | -5.946  | -15.731 | 1.00 | 24.60 |
| ATOM | 1581 | CB  | ALA | 173C | -31.310 | -3.645  | -13.840 | 1.00 | 22.16 |
| ATOM | 1582 | H   | ALA | 173C | -31.118 | -3.729  | -16.483 | 1.00 | 0.00  |
| ATOM | 1583 | N   | TYR | 173D | -31.565 | -6.776  | -13.834 | 1.00 | 23.00 |
| ATOM | 1584 | CA  | TYR | 173D | -32.398 | -7.967  | -13.709 | 1.00 | 23.15 |
| ATOM | 1585 | C   | TYR | 173D | -33.742 | -7.604  | -13.780 | 1.00 | 23.67 |
| ATOM | 1586 | O   | TYR | 173D | -34.718 | -8.333  | -13.31  | 1.00 | 25.70 |
| ATOM | 1587 | CB  | TYR | 173D | -31.707 | -8.996  | -12.301 | 1.00 | 22.72 |
| ATOM | 1588 | CG  | TYR | 173D | -30.513 | -9.713  | -13.402 | 1.00 | 22.59 |
| ATOM | 1589 | CD1 | TYR | 173D | -30.644 | -10.463 | -14.573 | 1.00 | 22.39 |
| ATOM | 1590 | CD2 | TYR | 173D | -29.263 | -9.675  | -12.779 | 1.00 | 21.99 |
| ATOM | 1591 | CE1 | TYR | 173D | -29.566 | -11.165 | -15.112 | 1.00 | 22.78 |
| ATOM | 1592 | CE2 | TYR | 173D | -28.172 | -10.379 | -13.311 | 1.00 | 23.40 |
| ATOM | 1593 | CZ  | TYR | 173D | -28.333 | -11.121 | -14.484 | 1.00 | 24.55 |
| ATOM | 1594 | OH  | TYR | 173D | -27.261 | -11.797 | -15.050 | 1.00 | 25.95 |
| ATOM | 1595 | H   | TYR | 173D | -30.815 | -6.671  | -13.223 | 1.00 | 0.00  |
| ATOM | 1596 | HH  | TYR | 173D | -27.539 | -12.256 | -15.865 | 1.00 | 0.00  |
| ATOM | 1597 | N   | THR | 173E | -33.777 | -6.491  | -12.352 | 1.00 | 23.43 |
| ATOM | 1598 | CA  | THR | 173E | -34.987 | -6.025  | -11.677 | 1.00 | 23.76 |
| ATOM | 1599 | C   | THR | 173E | -36.160 | -5.755  | -12.635 | 1.00 | 25.34 |
| ATOM | 1600 | O   | THR | 173E | -36.091 | -4.873  | -13.488 | 1.00 | 26.13 |
| ATOM | 1601 | CB  | THR | 173E | -34.691 | -4.740  | -10.877 | 1.00 | 21.96 |
| ATOM | 1602 | OG1 | THR | 173E | -33.419 | -4.865  | -10.231 | 1.00 | 21.26 |
| ATOM | 1603 | CG2 | THR | 173E | -35.753 | -4.503  | -9.825  | 1.00 | 20.44 |
| ATOM | 1604 | H   | THR | 173E | -32.974 | -5.951  | -12.256 | 1.00 | 0.00  |
| ATOM | 1605 | HG1 | THR | 173E | -33.479 | -5.537  | -9.537  | 1.00 | 0.00  |
| ATOM | 1606 | N   | GLY | 173F | -37.245 | -6.502  | -12.475 | 1.00 | 27.04 |
| ATOM | 1607 | CA  | GLY | 173F | -38.401 | -6.306  | -13.326 | 1.00 | 29.02 |
| ATOM | 1608 | C   | GLY | 173F | -38.864 | -4.861  | -13.304 | 1.00 | 30.11 |
| ATOM | 1609 | O   | GLY | 173F | -38.659 | -4.153  | -12.318 | 1.00 | 29.56 |
| ATOM | 1610 | H   | GLY | 173F | -37.257 | -7.149  | -11.737 | 1.00 | 0.00  |
| ATOM | 1611 | N   | ASP | 173G | -39.468 | -4.413  | -14.397 | 1.00 | 32.21 |
| ATOM | 1612 | CA  | ASP | 173G | -39.948 | -3.045  | -14.498 | 1.00 | 33.96 |
| ATOM | 1613 | C   | ASP | 173G | -41.110 | -2.692  | -13.580 | 1.00 | 34.60 |
| ATOM | 1614 | O   | ASP | 173G | -41.477 | -1.514  | -13.470 | 1.00 | 35.60 |
| ATOM | 1615 | CB  | ASP | 173G | -40.269 | -2.694  | -15.948 | 1.00 | 35.61 |
| ATOM | 1616 | CG  | ASP | 173G | -39.013 | -2.541  | -16.795 | 1.00 | 37.87 |
| ATOM | 1617 | OD1 | ASP | 173G | -38.642 | -1.381  | -17.110 | 1.00 | 38.56 |
| ATOM | 1618 | OD2 | ASP | 173G | -38.392 | -3.582  | -17.118 | 1.00 | 36.95 |

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|      |      |      |     |      |         |        |         |      |       |
|------|------|------|-----|------|---------|--------|---------|------|-------|
| ATOM | 1619 | H    | ASP | 173G | -39.537 | -4.977 | -15.195 | 1.00 | 0.00  |
| ATOM | 1620 | N    | ASP | 173H | -41.696 | -3.691 | -12.923 | 1.00 | 34.56 |
| ATOM | 1621 | CA   | ASP | 173H | -42.792 | -3.425 | -11.993 | 1.00 | 35.28 |
| ATOM | 1622 | C    | ASP | 173H | -42.216 | -2.953 | -10.657 | 1.00 | 33.17 |
| ATOM | 1623 | O    | ASP | 173H | -42.876 | -2.239 | -9.900  | 1.00 | 33.75 |
| ATOM | 1624 | CB   | ASP | 173H | -43.719 | -4.647 | -11.820 | 1.00 | 39.29 |
| ATOM | 1625 | CG   | ASP | 173H | -43.017 | -5.857 | -11.224 | 1.00 | 43.28 |
| ATOM | 1626 | OD1  | ASP | 173H | -43.093 | -6.047 | -9.987  | 1.00 | 44.47 |
| ATOM | 1627 | OD2  | ASP | 173H | -42.405 | -6.629 | -11.995 | 1.00 | 45.71 |
| ATOM | 1628 | H    | ASP | 173H | -41.435 | -4.628 | -13.053 | 1.00 | 0.00  |
| ATOM | 1629 | N    | VAL | 173I | -40.952 | -3.289 | -10.416 | 1.00 | 30.51 |
| ATOM | 1630 | CA   | VAL | 173I | -40.257 | -2.897 | -9.198  | 1.00 | 28.06 |
| ATOM | 1631 | C    | VAL | 173I | -39.718 | -1.476 | -9.364  | 1.00 | 29.63 |
| ATOM | 1632 | O    | VAL | 173I | -38.820 | -1.233 | -10.175 | 1.00 | 30.63 |
| ATOM | 1633 | CB   | VAL | 173I | -39.074 | -3.830 | -8.916  | 1.00 | 25.68 |
| ATOM | 1634 | CG1  | VAL | 173I | -38.437 | -3.482 | -7.584  | 1.00 | 25.28 |
| ATOM | 1635 | CG2  | VAL | 173I | -39.530 | -5.267 | -8.941  | 1.00 | 24.85 |
| ATOM | 1636 | H    | VAL | 173I | -40.462 | -3.827 | -11.072 | 1.00 | 0.00  |
| ATOM | 1637 | N    | ARG | 174  | -40.276 | -0.537 | -8.603  | 1.00 | 29.70 |
| ATOM | 1638 | CA   | ARG | 174  | -39.851 | 0.859  | -8.668  | 1.00 | 28.01 |
| ATOM | 1639 | C    | ARG | 174  | -38.492 | 1.006  | -8.000  | 1.00 | 24.47 |
| ATOM | 1640 | O    | ARG | 174  | -38.342 | 0.708  | -6.820  | 1.00 | 25.22 |
| ATOM | 1641 | CB   | ARG | 174  | -40.875 | 1.754  | -7.962  | 1.00 | 32.08 |
| ATOM | 1642 | CG   | ARG | 174  | -40.902 | 3.205  | -8.428  | 1.00 | 37.13 |
| ATOM | 1643 | CD   | ARG | 174  | -41.765 | 3.392  | -9.680  | 1.00 | 43.76 |
| ATOM | 1644 | NE   | ARG | 174  | -41.246 | 2.682  | -10.856 | 1.00 | 49.57 |
| ATOM | 1645 | CZ   | ARG | 174  | -41.842 | 1.642  | -11.449 | 1.00 | 51.72 |
| ATOM | 1646 | NH1  | ARG | 174  | -42.999 | 1.167  | -10.990 | 1.00 | 52.86 |
| ATOM | 1647 | NH2  | ARG | 174  | -41.267 | 1.058  | -12.496 | 1.00 | 52.80 |
| ATOM | 1648 | H    | ARG | 174  | -40.968 | -0.812 | -7.966  | 1.00 | 0.00  |
| ATOM | 1649 | HE   | ARG | 174  | -40.387 | 3.023  | -11.219 | 1.00 | 0.00  |
| ATOM | 1650 | HH11 | ARG | 174  | -43.446 | 1.570  | -10.192 | 1.00 | 0.00  |
| ATOM | 1651 | HH12 | ARG | 174  | -43.453 | 0.373  | -11.411 | 1.00 | 0.00  |
| ATOM | 1652 | HH21 | ARG | 174  | -40.380 | 1.444  | -12.791 | 1.00 | 0.00  |
| ATOM | 1653 | HH22 | ARG | 174  | -41.593 | 0.236  | -12.994 | 1.00 | 0.00  |
| ATOM | 1654 | N    | ILE | 175  | -37.500 | 1.438  | -8.760  | 1.00 | 21.33 |
| ATOM | 1655 | CA   | ILE | 175  | -36.162 | 1.625  | -8.230  | 1.00 | 18.97 |
| ATOM | 1656 | C    | ILE | 175  | -35.983 | 3.037  | -7.682  | 1.00 | 18.56 |
| ATOM | 1657 | O    | ILE | 175  | -35.505 | 3.196  | -6.561  | 1.00 | 19.95 |
| ATOM | 1658 | CB   | ILE | 175  | -35.101 | 1.277  | -9.278  | 1.00 | 18.53 |
| ATOM | 1659 | CG1  | ILE | 175  | -35.198 | -0.218 | -9.609  | 1.00 | 18.86 |
| ATOM | 1660 | CG2  | ILE | 175  | -33.728 | 1.619  | -8.765  | 1.00 | 18.13 |
| ATOM | 1661 | H    | ILE | 175  | -37.664 | 1.668  | -9.689  | 1.00 | 0.00  |
| ATOM | 1662 | CD   | ILE | 175  | -34.332 | -0.672 | -10.740 | 1.00 | 17.87 |
| ATOM | 1663 | N    | VAL | 176  | -36.342 | 4.068  | -8.442  | 1.00 | 17.12 |
| ATOM | 1664 | CA   | VAL | 176  | -36.218 | 5.412  | -7.891  | 1.00 | 18.02 |
| ATOM | 1665 | C    | VAL | 176  | -37.589 | 5.870  | -7.383  | 1.00 | 20.75 |
| ATOM | 1666 | O    | VAL | 176  | -38.509 | 6.159  | -8.156  | 1.00 | 21.89 |
| ATOM | 1667 | CB   | VAL | 176  | -35.538 | 6.442  | -8.854  | 1.00 | 15.79 |
| ATOM | 1668 | CG1  | VAL | 176  | -34.417 | 5.782  | -9.624  | 1.00 | 15.49 |
| ATOM | 1669 | CG2  | VAL | 176  | -36.524 | 7.120  | -9.762  | 1.00 | 13.99 |
| ATOM | 1670 | H    | VAL | 176  | -36.707 | 3.901  | -9.344  | 1.00 | 0.00  |
| ATOM | 1671 | N    | ARG | 177  | -37.735 | 5.853  | -6.060  | 1.00 | 21.95 |
| ATOM | 1672 | CA   | ARG | 177  | -38.984 | 6.225  | -5.399  | 1.00 | 21.76 |
| ATOM | 1673 | C    | ARG | 177  | -39.401 | 7.678  | -5.646  | 1.00 | 20.79 |
| ATOM | 1674 | O    | ARG | 177  | -38.619 | 8.490  | -6.134  | 1.00 | 21.17 |
| ATOM | 1675 | CB   | ARG | 177  | -38.874 | 5.981  | -3.889  | 1.00 | 23.66 |
| ATOM | 1676 | CG   | ARG | 177  | -38.101 | 4.728  | -3.468  | 1.00 | 26.30 |
| ATOM | 1677 | CD   | ARG | 177  | -38.721 | 3.453  | -4.004  | 1.00 | 29.29 |
| ATOM | 1678 | NE   | ARG | 177  | -38.762 | 2.396  | -2.993  | 1.00 | 32.19 |
| ATOM | 1679 | CZ   | ARG | 177  | -38.026 | 1.287  | -3.025  | 1.00 | 33.71 |
| ATOM | 1680 | NH1  | ARG | 177  | -37.170 | 1.080  | -4.019  | 1.00 | 33.86 |
| ATOM | 1681 | NH2  | ARG | 177  | -38.183 | 0.362  | -2.083  | 1.00 | 34.88 |

|      |      |      |     |     |         |        |         |      |       |
|------|------|------|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1682 | H    | ARG | 177 | -36.955 | 5.604  | -5.526  | 1.00 | 0.00  |
| ATOM | 1683 | HE   | ARG | 177 | -39.374 | 2.570  | -2.244  | 1.00 | 0.00  |
| ATOM | 1684 | HH11 | ARG | 177 | -37.064 | 1.758  | -4.751  | 1.00 | 0.00  |
| ATOM | 1685 | HH12 | ARG | 177 | -36.538 | 0.309  | -4.128  | 1.00 | 0.00  |
| ATOM | 1686 | HH21 | ARG | 177 | -38.847 | 0.479  | -1.345  | 1.00 | 0.00  |
| ATOM | 1687 | HH22 | ARG | 177 | -37.629 | -0.468 | -2.105  | 1.00 | 0.00  |
| ATOM | 1688 | N    | ASP | 178 | -40.630 | 7.999  | -5.262  | 1.00 | 20.04 |
| ATOM | 1689 | CA   | ASP | 178 | -41.191 | 9.336  | -5.418  | 1.00 | 18.15 |
| ATOM | 1690 | C    | ASP | 178 | -40.471 | 10.413 | -4.620  | 1.00 | 15.72 |
| ATOM | 1691 | O    | ASP | 178 | -40.574 | 11.595 | -4.935  | 1.00 | 15.89 |
| ATOM | 1692 | CB   | ASP | 178 | -42.658 | 9.327  | -5.004  | 1.00 | 21.04 |
| ATOM | 1693 | CG   | ASP | 178 | -43.567 | 8.848  | -6.098  | 1.00 | 24.50 |
| ATOM | 1694 | OD1  | ASP | 178 | -43.420 | 7.698  | -6.575  | 1.00 | 26.28 |
| ATOM | 1695 | OD2  | ASP | 178 | -44.455 | 9.635  | -6.484  | 1.00 | 27.33 |
| ATOM | 1696 | H    | ASP | 178 | -41.228 | 7.329  | -4.875  | 1.00 | 0.00  |
| ATOM | 1697 | N    | ASP | 179 | -39.783 | 10.020 | -3.558  | 1.00 | 14.11 |
| ATOM | 1698 | CA   | ASP | 179 | -39.071 | 10.981 | -2.731  | 1.00 | 12.77 |
| ATOM | 1699 | C    | ASP | 179 | -37.677 | 11.268 | -3.244  | 1.00 | 11.77 |
| ATOM | 1700 | O    | ASP | 179 | -36.926 | 12.009 | -2.623  | 1.00 | 11.43 |
| ATOM | 1701 | CB   | ASP | 179 | -39.013 | 10.513 | -1.276  | 1.00 | 14.68 |
| ATOM | 1702 | CG   | ASP | 179 | -38.320 | 9.178  | -1.112  | 1.00 | 15.98 |
| ATOM | 1703 | OD1  | ASP | 179 | -38.815 | 8.170  | -1.655  | 1.00 | 17.32 |
| ATOM | 1704 | OD2  | ASP | 179 | -37.291 | 9.125  | -0.412  | 1.00 | 16.93 |
| ATOM | 1705 | H    | ASP | 179 | -39.761 | 9.075  | -3.290  | 1.00 | 0.00  |
| ATOM | 1706 | N    | MET | 180 | -37.351 | 10.726 | -4.412  | 1.00 | 12.30 |
| ATOM | 1707 | CA   | MET | 180 | -36.039 | 10.925 | -5.017  | 1.00 | 11.45 |
| ATOM | 1708 | C    | MET | 180 | -36.146 | 11.779 | -6.268  | 1.00 | 13.26 |
| ATOM | 1709 | O    | MET | 180 | -37.229 | 11.961 | -6.824  | 1.00 | 14.48 |
| ATOM | 1710 | CB   | MET | 180 | -35.414 | 9.579  | -5.357  | 1.00 | 9.46  |
| ATOM | 1711 | CG   | MET | 180 | -35.427 | 8.619  | -4.197  | 1.00 | 8.00  |
| ATOM | 1712 | SD   | MET | 180 | -34.848 | 7.020  | -4.652  | 1.00 | 8.13  |
| ATOM | 1713 | CE   | MET | 180 | -34.880 | 6.211  | -3.094  | 1.00 | 8.00  |
| ATOM | 1714 | H    | MET | 180 | -37.994 | 10.183 | -4.906  | 1.00 | 0.00  |
| ATOM | 1715 | N    | LEU | 181 | -35.017 | 12.324 | -6.689  | 1.00 | 15.44 |
| ATOM | 1716 | CA   | LEU | 181 | -34.937 | 13.179 | -7.864  | 1.00 | 17.08 |
| ATOM | 1717 | C    | LEU | 181 | -33.682 | 12.757 | -8.627  | 1.00 | 18.68 |
| ATOM | 1718 | O    | LEU | 181 | -32.717 | 12.297 | -8.019  | 1.00 | 19.99 |
| ATOM | 1719 | CB   | LEU | 181 | -34.853 | 14.650 | -7.412  | 1.00 | 16.58 |
| ATOM | 1720 | CG   | LEU | 181 | -34.544 | 15.785 | -8.399  | 1.00 | 17.04 |
| ATOM | 1721 | CD1  | LEU | 181 | -35.107 | 17.098 | -7.902  | 1.00 | 17.23 |
| ATOM | 1722 | CD2  | LEU | 181 | -33.055 | 15.915 | -8.600  | 1.00 | 17.26 |
| ATOM | 1723 | H    | LEU | 181 | -34.199 | 12.161 | -6.179  | 1.00 | 0.00  |
| ATOM | 1724 | N    | CYS | 182 | -33.702 | 12.873 | -9.950  | 1.00 | 18.96 |
| ATOM | 1725 | CA   | CYS | 182 | -32.551 | 12.494 | -10.747 | 1.00 | 19.50 |
| ATOM | 1726 | C    | CYS | 182 | -31.983 | 13.662 | -11.504 | 1.00 | 21.31 |
| ATOM | 1727 | O    | CYS | 182 | -32.720 | 14.528 | -11.982 | 1.00 | 22.70 |
| ATOM | 1728 | CB   | CYS | 182 | -32.921 | 11.423 | -11.738 | 1.00 | 19.26 |
| ATOM | 1729 | SG   | CYS | 182 | -33.455 | 9.889  | -10.953 | 1.00 | 22.46 |
| ATOM | 1730 | H    | CYS | 182 | -34.483 | 13.224 | -10.421 | 1.00 | 0.00  |
| ATOM | 1731 | N    | ALA | 183 | -30.668 | 13.654 | -11.641 | 1.00 | 21.56 |
| ATOM | 1732 | CA   | ALA | 183 | -29.958 | 14.696 | -12.344 | 1.00 | 22.35 |
| ATOM | 1733 | C    | ALA | 183 | -28.574 | 14.167 | -12.689 | 1.00 | 25.09 |
| ATOM | 1734 | O    | ALA | 183 | -28.089 | 13.211 | -12.077 | 1.00 | 25.38 |
| ATOM | 1735 | CB   | ALA | 183 | -29.857 | 15.933 | -11.473 | 1.00 | 20.35 |
| ATOM | 1736 | H    | ALA | 183 | -30.153 | 12.927 | -11.220 | 1.00 | 0.00  |
| ATOM | 1737 | N    | GLY | 184 | -27.960 | 14.764 | -13.702 | 1.00 | 27.62 |
| ATOM | 1738 | CA   | GLY | 184 | -26.636 | 14.344 | -14.112 | 1.00 | 28.49 |
| ATOM | 1739 | C    | GLY | 184 | -26.672 | 13.504 | -15.369 | 1.00 | 29.74 |
| ATOM | 1740 | O    | GLY | 184 | -27.743 | 13.117 | -15.856 | 1.00 | 29.35 |
| ATOM | 1741 | H    | GLY | 184 | -28.470 | 15.423 | -14.213 | 1.00 | 0.00  |
| ATOM | 1742 | N    | ASN | 185 | -25.489 | 13.225 | -15.899 | 1.00 | 30.82 |
| ATOM | 1743 | CA   | ASN | 185 | -25.357 | 12.434 | -17.107 | 1.00 | 31.75 |
| ATOM | 1744 | C    | ASN | 185 | -24.021 | 11.718 | -17.121 | 1.00 | 32.71 |

|      |      |      |     |     |         |        |         |      |       |
|------|------|------|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1745 | O    | ASN | 185 | -23.272 | 11.753 | -16.142 | 1.00 | 32.76 |
| ATOM | 1746 | CB   | ASN | 185 | -25.507 | 13.316 | -18.356 | 1.00 | 31.87 |
| ATOM | 1747 | CG   | ASN | 185 | -24.467 | 14.418 | -18.427 | 1.00 | 31.07 |
| ATOM | 1748 | OD1  | ASN | 185 | -23.343 | 14.253 | -17.973 | 1.00 | 31.05 |
| ATOM | 1749 | ND2  | ASN | 185 | -24.836 | 15.541 | -19.023 | 1.00 | 31.34 |
| ATOM | 1750 | H    | ASN | 185 | -24.680 | 13.513 | -15.432 | 1.00 | 0.00  |
| ATOM | 1751 | HD21 | ASN | 185 | -25.748 | 15.588 | -19.376 | 1.00 | 0.00  |
| ATOM | 1752 | HD22 | ASN | 185 | -24.171 | 16.253 | -19.082 | 1.00 | 0.00  |
| ATOM | 1753 | N    | THR | 186 | -23.692 | 11.144 | -18.270 | 1.00 | 33.84 |
| ATOM | 1754 | CA   | THR | 186 | -22.459 | 10.393 | -18.449 | 1.00 | 34.53 |
| ATOM | 1755 | C    | THR | 186 | -21.183 | 11.249 | -18.532 | 1.00 | 36.08 |
| ATOM | 1756 | O    | THR | 186 | -20.119 | 10.739 | -18.886 | 1.00 | 37.14 |
| ATOM | 1757 | CB   | THR | 186 | -22.579 | 9.504  | -19.703 | 1.00 | 33.21 |
| ATOM | 1758 | OG1  | THR | 186 | -21.572 | 8.490  | -19.683 | 1.00 | 34.42 |
| ATOM | 1759 | CG2  | THR | 186 | -22.438 | 10.335 | -20.962 | 1.00 | 34.10 |
| ATOM | 1760 | H    | THR | 186 | -24.296 | 11.210 | -19.033 | 1.00 | 0.00  |
| ATOM | 1761 | HG1  | THR | 186 | -20.708 | 8.907  | -19.523 | 1.00 | 0.00  |
| ATOM | 1762 | N    | ARG | 187 | -21.286 | 12.538 | -18.205 | 1.00 | 36.29 |
| ATOM | 1763 | CA   | ARG | 187 | -20.144 | 13.451 | -18.261 | 1.00 | 36.05 |
| ATOM | 1764 | C    | ARG | 187 | -20.161 | 14.441 | -17.110 | 1.00 | 34.58 |
| ATOM | 1765 | O    | ARG | 187 | -19.230 | 15.224 | -16.955 | 1.00 | 35.60 |
| ATOM | 1766 | CB   | ARG | 187 | -20.144 | 14.249 | -19.571 | 1.00 | 39.86 |
| ATOM | 1767 | CG   | ARG | 187 | -20.060 | 13.416 | -20.841 | 1.00 | 45.36 |
| ATOM | 1768 | CD   | ARG | 187 | -20.150 | 14.281 | -22.095 | 1.00 | 49.61 |
| ATOM | 1769 | NE   | ARG | 187 | -20.186 | 13.462 | -23.310 | 1.00 | 54.73 |
| ATOM | 1770 | CZ   | ARG | 187 | -19.491 | 13.712 | -24.421 | 1.00 | 56.94 |
| ATOM | 1771 | NH1  | ARG | 187 | -18.690 | 14.773 | -24.492 | 1.00 | 58.03 |
| ATOM | 1772 | NH2  | ARG | 187 | -19.590 | 12.889 | -25.464 | 1.00 | 57.38 |
| ATOM | 1773 | H    | ARG | 187 | -22.126 | 12.901 | -17.895 | 1.00 | 0.00  |
| ATOM | 1774 | HE   | ARG | 187 | -20.782 | 12.681 | -23.245 | 1.00 | 0.00  |
| ATOM | 1775 | HH11 | ARG | 187 | -18.608 | 15.389 | -23.701 | 1.00 | 0.00  |
| ATOM | 1776 | HH12 | ARG | 187 | -18.142 | 15.011 | -25.296 | 1.00 | 0.00  |
| ATOM | 1777 | HH21 | ARG | 187 | -20.185 | 12.083 | -25.418 | 1.00 | 0.00  |
| ATOM | 1778 | HH22 | ARG | 187 | -19.087 | 13.041 | -26.318 | 1.00 | 0.00  |
| ATOM | 1779 | N    | ARG | 188 | -21.238 | 14.450 | -16.339 | 1.00 | 32.47 |
| ATOM | 1780 | CA   | ARG | 188 | -21.368 | 15.366 | -15.215 | 1.00 | 30.59 |
| ATOM | 1781 | C    | ARG | 188 | -22.214 | 14.684 | -14.164 | 1.00 | 27.24 |
| ATOM | 1782 | O    | ARG | 188 | -23.273 | 14.153 | -14.487 | 1.00 | 26.98 |
| ATOM | 1783 | CB   | ARG | 188 | -22.078 | 16.645 | -15.656 | 1.00 | 34.39 |
| ATOM | 1784 | CG   | ARG | 188 | -21.505 | 17.304 | -16.888 | 1.00 | 39.02 |
| ATOM | 1785 | CD   | ARG | 188 | -22.201 | 18.612 | -17.142 | 1.00 | 44.49 |
| ATOM | 1786 | NE   | ARG | 188 | -22.037 | 19.065 | -18.517 | 1.00 | 50.18 |
| ATOM | 1787 | CZ   | ARG | 188 | -23.018 | 19.590 | -19.248 | 1.00 | 53.82 |
| ATOM | 1788 | NH1  | ARG | 188 | -24.238 | 19.726 | -18.724 | 1.00 | 54.77 |
| ATOM | 1789 | NH2  | ARG | 188 | -22.781 | 19.988 | -20.497 | 1.00 | 55.95 |
| ATOM | 1790 | H    | ARG | 188 | -21.994 | 13.852 | -16.502 | 1.00 | 0.00  |
| ATOM | 1791 | HE   | ARG | 188 | -21.117 | 18.948 | -18.849 | 1.00 | 0.00  |
| ATOM | 1792 | HH11 | ARG | 188 | -24.369 | 19.477 | -17.753 | 1.00 | 0.00  |
| ATOM | 1793 | HH12 | ARG | 188 | -25.020 | 20.118 | -19.211 | 1.00 | 0.00  |
| ATOM | 1794 | HH21 | ARG | 188 | -21.864 | 19.906 | -20.897 | 1.00 | 0.00  |
| ATOM | 1795 | HH22 | ARG | 188 | -23.497 | 20.392 | -21.075 | 1.00 | 0.00  |
| ATOM | 1796 | N    | ASP | 189 | -21.790 | 14.765 | -12.910 | 1.00 | 24.34 |
| ATOM | 1797 | CA   | ASP | 189 | -22.509 | 14.123 | -11.816 | 1.00 | 22.44 |
| ATOM | 1798 | C    | ASP | 189 | -21.759 | 14.378 | -10.521 | 1.00 | 22.01 |
| ATOM | 1799 | O    | ASP | 189 | -20.601 | 14.789 | -10.546 | 1.00 | 21.55 |
| ATOM | 1800 | CB   | ASP | 189 | -22.550 | 12.609 | -12.081 | 1.00 | 21.45 |
| ATOM | 1801 | CG   | ASP | 189 | -23.253 | 11.819 | -10.985 | 1.00 | 21.83 |
| ATOM | 1802 | OD1  | ASP | 189 | -24.068 | 12.380 | -10.222 | 1.00 | 24.61 |
| ATOM | 1803 | OD2  | ASP | 189 | -22.999 | 10.605 | -10.906 | 1.00 | 19.74 |
| ATOM | 1804 | H    | ASP | 189 | -20.960 | 15.245 | -12.703 | 1.00 | 0.00  |
| ATOM | 1805 | N    | SER | 190 | -22.441 | 14.224 | -9.393  | 1.00 | 22.95 |
| ATOM | 1806 | CA   | SER | 190 | -21.792 | 14.370 | -8.096  | 1.00 | 23.82 |
| ATOM | 1807 | C    | SER | 190 | -21.041 | 13.045 | -7.926  | 1.00 | 24.53 |

|      |      |      |     |     |         |        |        |      |       |
|------|------|------|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1808 | O    | SER | 190 | -21.179 | 12.146 | -8.757 | 1.00 | 25.46 |
| ATOM | 1809 | CB   | SER | 190 | -22.823 | 14.573 | -6.972 | 1.00 | 23.32 |
| ATOM | 1810 | OG   | SER | 190 | -23.736 | 13.491 | -6.845 | 1.00 | 22.29 |
| ATOM | 1811 | H    | SER | 190 | -23.390 | 13.989 | -9.443 | 1.00 | 0.00  |
| ATOM | 1812 | HG   | SER | 190 | -23.975 | 13.143 | -7.725 | 1.00 | 0.00  |
| ATOM | 1813 | N    | CYS | 191 | -20.243 | 12.907 | -6.881 | 1.00 | 23.49 |
| ATOM | 1814 | CA   | CYS | 191 | -19.514 | 11.670 | -6.712 | 1.00 | 22.82 |
| ATOM | 1815 | C    | CYS | 191 | -19.243 | 11.399 | -5.236 | 1.00 | 23.00 |
| ATOM | 1816 | O    | CYS | 191 | -19.813 | 12.055 | -4.361 | 1.00 | 23.19 |
| ATOM | 1817 | CB   | CYS | 191 | -18.231 | 11.710 | -7.550 | 1.00 | 21.77 |
| ATOM | 1818 | SG   | CYS | 191 | -17.409 | 10.103 | -7.803 | 1.00 | 23.53 |
| ATOM | 1819 | H    | CYS | 191 | -20.140 | 13.606 | -6.214 | 1.00 | 0.00  |
| ATOM | 1820 | N    | GLN | 192 | -18.418 | 10.396 | -4.958 | 1.00 | 23.12 |
| ATOM | 1821 | CA   | GLN | 192 | -18.091 | 10.019 | -3.589 | 1.00 | 23.66 |
| ATOM | 1822 | C    | GLN | 192 | -17.583 | 11.218 | -2.812 | 1.00 | 22.07 |
| ATOM | 1823 | O    | GLN | 192 | -16.638 | 11.867 | -3.234 | 1.00 | 23.86 |
| ATOM | 1824 | CB   | GLN | 192 | -17.016 | 8.936  | -3.596 | 1.00 | 28.11 |
| ATOM | 1825 | CG   | GLN | 192 | -16.881 | 8.173  | -2.292 | 1.00 | 34.86 |
| ATOM | 1826 | CD   | GLN | 192 | -18.060 | 7.252  | -2.036 | 1.00 | 40.16 |
| ATOM | 1827 | OE1  | GLN | 192 | -18.835 | 7.460  | -1.099 | 1.00 | 42.98 |
| ATOM | 1828 | NE2  | GLN | 192 | -18.207 | 6.229  | -2.876 | 1.00 | 42.25 |
| ATOM | 1829 | H    | GLN | 192 | -17.990 | 9.901  | -5.689 | 1.00 | 0.00  |
| ATOM | 1830 | HE21 | GLN | 192 | -17.554 | 6.114  | -3.599 | 1.00 | 0.00  |
| ATOM | 1831 | HE22 | GLN | 192 | -18.971 | 5.635  | -2.719 | 1.00 | 0.00  |
| ATOM | 1832 | N    | GLY | 193 | -18.229 | 11.533 | -1.698 | 1.00 | 19.90 |
| ATOM | 1833 | CA   | GLY | 193 | -17.784 | 12.655 | -0.894 | 1.00 | 18.35 |
| ATOM | 1834 | C    | GLY | 193 | -18.614 | 13.911 | -1.035 | 1.00 | 17.76 |
| ATOM | 1835 | O    | GLY | 193 | -18.389 | 14.877 | -0.296 | 1.00 | 19.03 |
| ATOM | 1836 | H    | GLY | 193 | -19.016 | 11.023 | -1.421 | 1.00 | 0.00  |
| ATOM | 1837 | N    | ASP | 194 | -19.524 | 13.926 | -2.007 | 1.00 | 16.45 |
| ATOM | 1838 | CA   | ASP | 194 | -20.407 | 15.068 | -2.221 | 1.00 | 15.06 |
| ATOM | 1839 | C    | ASP | 194 | -21.717 | 14.857 | -1.484 | 1.00 | 14.80 |
| ATOM | 1840 | O    | ASP | 194 | -22.484 | 15.798 | -1.308 | 1.00 | 15.38 |
| ATOM | 1841 | CB   | ASP | 194 | -20.705 | 15.258 | -3.703 | 1.00 | 15.50 |
| ATOM | 1842 | CG   | ASP | 194 | -19.497 | 15.689 | -4.487 | 1.00 | 16.66 |
| ATOM | 1843 | OD1  | ASP | 194 | -18.741 | 16.561 | -4.004 | 1.00 | 18.05 |
| ATOM | 1844 | OD2  | ASP | 194 | -19.296 | 15.154 | -5.595 | 1.00 | 15.67 |
| ATOM | 1845 | H    | ASP | 194 | -19.619 | 13.193 | -2.652 | 1.00 | 0.00  |
| ATOM | 1846 | N    | SER | 195 | -21.965 | 13.618 | -1.061 | 1.00 | 14.17 |
| ATOM | 1847 | CA   | SER | 195 | -23.173 | 13.247 | -0.331 | 1.00 | 14.15 |
| ATOM | 1848 | C    | SER | 195 | -23.517 | 14.283 | 0.713  | 1.00 | 15.35 |
| ATOM | 1849 | O    | SER | 195 | -22.626 | 14.848 | 1.339  | 1.00 | 17.03 |
| ATOM | 1850 | CB   | SER | 195 | -22.999 | 11.892 | 0.339  | 1.00 | 14.32 |
| ATOM | 1851 | OG   | SER | 195 | -23.149 | 10.834 | -0.598 | 1.00 | 16.17 |
| ATOM | 1852 | H    | SER | 195 | -21.281 | 12.979 | -1.252 | 1.00 | 0.00  |
| ATOM | 1853 | N    | GLY | 196 | -24.807 | 14.559 | 0.869  | 1.00 | 16.19 |
| ATOM | 1854 | CA   | GLY | 196 | -25.247 | 15.557 | 1.828  | 1.00 | 16.95 |
| ATOM | 1855 | C    | GLY | 196 | -25.215 | 16.953 | 1.234  | 1.00 | 19.53 |
| ATOM | 1856 | O    | GLY | 196 | -25.832 | 17.876 | 1.773  | 1.00 | 22.52 |
| ATOM | 1857 | H    | GLY | 196 | -25.457 | 14.063 | 0.327  | 1.00 | 0.00  |
| ATOM | 1858 | N    | GLY | 197 | -24.520 | 17.101 | 0.107  | 1.00 | 19.48 |
| ATOM | 1859 | CA   | GLY | 197 | -24.402 | 18.388 | -0.564 | 1.00 | 17.72 |
| ATOM | 1860 | C    | GLY | 197 | -25.663 | 18.813 | -1.285 | 1.00 | 16.98 |
| ATOM | 1861 | O    | GLY | 197 | -26.482 | 17.977 | -1.656 | 1.00 | 17.29 |
| ATOM | 1862 | H    | GLY | 197 | -24.047 | 16.363 | -0.314 | 1.00 | 0.00  |
| ATOM | 1863 | N    | PRO | 198 | -25.831 | 20.116 | -1.518 | 1.00 | 17.20 |
| ATOM | 1864 | CA   | PRO | 198 | -26.994 | 20.681 | -2.196 | 1.00 | 17.64 |
| ATOM | 1865 | C    | PRO | 198 | -26.993 | 20.682 | -3.720 | 1.00 | 18.82 |
| ATOM | 1866 | O    | PRO | 198 | -25.971 | 20.943 | -4.353 | 1.00 | 20.26 |
| ATOM | 1867 | CB   | PRO | 198 | -26.991 | 22.119 | -1.686 | 1.00 | 17.40 |
| ATOM | 1868 | CG   | PRO | 198 | -25.541 | 22.432 | -1.642 | 1.00 | 15.54 |
| ATOM | 1869 | CD   | PRO | 198 | -24.992 | 21.190 | -0.954 | 1.00 | 17.43 |
| ATOM | 1870 | N    | LEU | 199 | -28.151 | 20.379 | -4.296 | 1.00 | 20.11 |

|      |      |      |     |     |         |        |         |      |       |
|------|------|------|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1871 | CA   | LEU | 199 | -28.354 | 20.435 | -5.740  | 1.00 | 20.15 |
| ATOM | 1872 | C    | LEU | 199 | -29.300 | 21.614 | -5.840  | 1.00 | 21.06 |
| ATOM | 1373 | O    | LEU | 199 | -30.475 | 21.503 | -5.484  | 1.00 | 20.83 |
| ATOM | 1874 | CB   | LEU | 199 | -29.057 | 19.185 | -6.275  | 1.00 | 19.27 |
| ATOM | 1875 | CG   | LEU | 199 | -29.697 | 19.349 | -7.665  | 1.00 | 18.76 |
| ATOM | 1376 | CD1  | LEU | 199 | -28.667 | 19.670 | -8.723  | 1.00 | 18.01 |
| ATOM | 1877 | CD2  | LEU | 199 | -30.434 | 18.094 | -8.047  | 1.00 | 19.55 |
| ATOM | 1878 | H    | LEU | 199 | -28.885 | 20.069 | -3.724  | 1.00 | 0.00  |
| ATOM | 1879 | N    | VAL | 200 | -28.777 | 22.760 | -6.246  | 1.00 | 22.37 |
| ATOM | 1880 | CA   | VAL | 200 | -29.592 | 23.962 | -6.358  | 1.00 | 23.26 |
| ATOM | 1881 | C    | VAL | 200 | -30.021 | 24.242 | -7.789  | 1.00 | 23.81 |
| ATOM | 1882 | O    | VAL | 200 | -29.437 | 23.714 | -8.732  | 1.00 | 24.03 |
| ATOM | 1883 | CB   | VAL | 200 | -28.846 | 25.183 | -5.809  | 1.00 | 23.69 |
| ATOM | 1884 | CG1  | VAL | 200 | -28.614 | 25.020 | -4.312  | 1.00 | 22.32 |
| ATOM | 1885 | CG2  | VAL | 200 | -27.518 | 25.363 | -6.553  | 1.00 | 24.45 |
| ATOM | 1886 | H    | VAL | 200 | -27.845 | 22.737 | -6.552  | 1.00 | 0.00  |
| ATOM | 1887 | N    | CYS | 201 | -31.053 | 25.064 | -7.939  | 1.00 | 24.78 |
| ATOM | 1888 | CA   | CYS | 201 | -31.569 | 25.443 | -9.247  | 1.00 | 25.34 |
| ATOM | 1889 | C    | CYS | 201 | -32.029 | 26.884 | -9.185  | 1.00 | 27.18 |
| ATOM | 1890 | O    | CYS | 201 | -32.536 | 27.346 | -8.157  | 1.00 | 27.06 |
| ATOM | 1891 | CB   | CYS | 201 | -32.748 | 24.568 | -9.633  | 1.00 | 24.01 |
| ATOM | 1892 | SG   | CYS | 201 | -32.401 | 22.798 | -9.499  | 1.00 | 24.78 |
| ATOM | 1893 | H    | CYS | 201 | -31.511 | 25.388 | -7.139  | 1.00 | 0.00  |
| ATOM | 1894 | N    | LYS | 202 | -31.813 | 27.607 | -10.273 | 1.00 | 29.46 |
| ATOM | 1895 | CA   | LYS | 202 | -32.209 | 28.999 | -10.337 | 1.00 | 32.31 |
| ATOM | 1896 | C    | LYS | 202 | -33.624 | 29.049 | -10.887 | 1.00 | 34.40 |
| ATOM | 1897 | O    | LYS | 202 | -33.823 | 29.045 | -12.103 | 1.00 | 34.96 |
| ATOM | 1898 | CB   | LYS | 202 | -31.236 | 29.789 | -11.216 | 1.00 | 33.16 |
| ATOM | 1899 | CG   | LYS | 202 | -31.383 | 31.301 | -11.118 | 1.00 | 36.87 |
| ATOM | 1900 | CD   | LYS | 202 | -30.050 | 32.033 | -11.344 | 1.00 | 39.46 |
| ATOM | 1901 | CE   | LYS | 202 | -29.446 | 31.789 | -12.735 | 1.00 | 42.10 |
| ATOM | 1902 | NZ   | LYS | 202 | -30.239 | 32.373 | -13.871 | 1.00 | 44.87 |
| ATOM | 1903 | H    | LYS | 202 | -31.404 | 27.150 | -11.040 | 1.00 | 0.00  |
| ATOM | 1904 | HZ1  | LYS | 202 | -30.307 | 33.403 | -13.751 | 1.00 | 0.00  |
| ATOM | 1905 | HZ2  | LYS | 202 | -31.190 | 31.952 | -13.882 | 1.00 | 0.00  |
| ATOM | 1906 | HZ3  | LYS | 202 | -29.757 | 32.155 | -14.768 | 1.00 | 0.00  |
| ATOM | 1907 | N    | VAL | 203 | -34.601 | 29.026 | -9.984  | 1.00 | 36.68 |
| ATOM | 1908 | CA   | VAL | 203 | -36.014 | 29.067 | -10.353 | 1.00 | 38.86 |
| ATOM | 1909 | C    | VAL | 203 | -36.563 | 30.477 | -10.187 | 1.00 | 41.61 |
| ATOM | 1910 | O    | VAL | 203 | -36.651 | 30.992 | -9.071  | 1.00 | 41.93 |
| ATOM | 1911 | CB   | VAL | 203 | -36.857 | 28.099 | -9.496  | 1.00 | 37.56 |
| ATOM | 1912 | CG1  | VAL | 203 | -38.336 | 28.267 | -9.803  | 1.00 | 37.29 |
| ATOM | 1913 | CG2  | VAL | 203 | -36.438 | 26.680 | -9.765  | 1.00 | 38.59 |
| ATOM | 1914 | H    | VAL | 203 | -34.348 | 29.049 | -9.033  | 1.00 | 0.00  |
| ATOM | 1915 | N    | ASN | 204 | -36.927 | 31.095 | -11.308 | 1.00 | 44.67 |
| ATOM | 1916 | CA   | ASN | 204 | -37.468 | 32.452 | -11.313 | 1.00 | 47.09 |
| ATOM | 1917 | C    | ASN | 204 | -36.478 | 33.431 | -10.672 | 1.00 | 46.66 |
| ATOM | 1918 | O    | ASN | 204 | -36.812 | 34.147 | -9.729  | 1.00 | 46.64 |
| ATOM | 1919 | CB   | ASN | 204 | -38.820 | 32.486 | -10.582 | 1.00 | 50.73 |
| ATOM | 1920 | CG   | ASN | 204 | -39.581 | 33.790 | -10.801 | 1.00 | 54.29 |
| ATOM | 1921 | OD1  | ASN | 204 | -39.253 | 34.578 | -11.693 | 1.00 | 55.94 |
| ATOM | 1922 | ND2  | ASN | 204 | -40.623 | 34.008 | -9.999  | 1.00 | 55.44 |
| ATOM | 1923 | H    | ASN | 204 | -36.828 | 30.624 | -12.159 | 1.00 | 0.00  |
| ATOM | 1924 | HD21 | ASN | 204 | -40.851 | 33.345 | -9.317  | 1.00 | 0.00  |
| ATOM | 1925 | HD22 | ASN | 204 | -41.101 | 34.848 | -10.144 | 1.00 | 0.00  |
| ATOM | 1926 | N    | GLY | 205 | -35.237 | 33.402 | -11.153 | 1.00 | 46.17 |
| ATOM | 1927 | CA   | GLY | 205 | -34.210 | 34.294 | -10.636 | 1.00 | 46.09 |
| ATOM | 1928 | C    | GLY | 205 | -33.576 | 33.960 | -9.290  | 1.00 | 45.77 |
| ATOM | 1929 | O    | GLY | 205 | -32.503 | 34.476 | -8.964  | 1.00 | 46.28 |
| ATOM | 1930 | H    | GLY | 205 | -35.033 | 32.759 | -11.856 | 1.00 | 0.00  |
| ATOM | 1931 | N    | THR | 206 | -34.213 | 33.105 | -8.502  | 1.00 | 44.07 |
| ATOM | 1932 | CA   | THR | 206 | -33.664 | 32.749 | -7.204  | 1.00 | 41.60 |
| ATOM | 1933 | C    | THR | 206 | -33.090 | 31.330 | -7.130  | 1.00 | 38.47 |

|      |      |      |     |     |         |        |        |      |       |
|------|------|------|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1934 | O    | THR | 206 | -33.393 | 30.470 | -7.967 | 1.00 | 36.60 |
| ATOM | 1935 | CB   | THR | 206 | -34.700 | 32.987 | -6.084 | 1.00 | 42.90 |
| ATOM | 1936 | OG1  | THR | 206 | -35.980 | 32.478 | -6.488 | 1.00 | 44.64 |
| ATOM | 1937 | CG2  | THR | 206 | -34.828 | 34.475 | -5.800 | 1.00 | 43.50 |
| ATOM | 1938 | H    | THR | 206 | -35.082 | 32.705 | -8.730 | 1.00 | 0.00  |
| ATOM | 1939 | HG1  | THR | 206 | -36.583 | 32.516 | -5.736 | 1.00 | 0.00  |
| ATOM | 1940 | N    | TRP | 207 | -32.211 | 31.123 | -6.151 | 1.00 | 35.21 |
| ATOM | 1941 | CA   | TRP | 207 | -31.566 | 29.835 | -5.922 | 1.00 | 30.48 |
| ATOM | 1942 | C    | TRP | 207 | -32.353 | 29.030 | -4.913 | 1.00 | 27.89 |
| ATOM | 1943 | O    | TRP | 207 | -32.456 | 29.410 | -3.738 | 1.00 | 27.82 |
| ATOM | 1944 | CB   | TRP | 207 | -30.146 | 30.028 | -5.388 | 1.00 | 28.99 |
| ATOM | 1945 | CG   | TRP | 207 | -29.141 | 30.331 | -6.437 | 1.00 | 26.88 |
| ATOM | 1946 | CD1  | TRP | 207 | -28.345 | 31.432 | -6.515 | 1.00 | 27.09 |
| ATOM | 1947 | CD2  | TRP | 207 | -28.813 | 29.516 | -7.562 | 1.00 | 25.96 |
| ATOM | 1948 | NE1  | TRP | 207 | -27.538 | 31.352 | -7.622 | 1.00 | 27.02 |
| ATOM | 1949 | CE2  | TRP | 207 | -27.807 | 30.186 | -8.284 | 1.00 | 25.40 |
| ATOM | 1950 | CE3  | TRP | 207 | -29.271 | 28.281 | -8.030 | 1.00 | 26.67 |
| ATOM | 1951 | CZ2  | TRP | 207 | -27.252 | 29.665 | -9.449 | 1.00 | 26.59 |
| ATOM | 1952 | CZ3  | TRP | 207 | -28.720 | 27.759 | -9.189 | 1.00 | 27.44 |
| ATOM | 1953 | CH2  | TRP | 207 | -27.721 | 28.452 | -9.886 | 1.00 | 27.93 |
| ATOM | 1954 | H    | TRP | 207 | -31.995 | 31.863 | -5.555 | 1.00 | 0.00  |
| ATOM | 1955 | HE1  | TRP | 207 | -26.869 | 32.027 | -7.859 | 1.00 | 0.00  |
| ATOM | 1956 | N    | LEU | 208 | -32.932 | 27.936 | -5.380 | 1.00 | 23.96 |
| ATOM | 1957 | CA   | LEU | 208 | -33.702 | 27.066 | -4.515 | 1.00 | 20.83 |
| ATOM | 1958 | C    | LEU | 208 | -32.956 | 25.758 | -4.465 | 1.00 | 19.72 |
| ATOM | 1959 | O    | LEU | 208 | -32.316 | 25.372 | -5.442 | 1.00 | 20.15 |
| ATOM | 1960 | CB   | LEU | 208 | -35.083 | 26.805 | -5.105 | 1.00 | 19.19 |
| ATOM | 1961 | CG   | LEU | 208 | -35.981 | 27.989 | -5.421 | 1.00 | 17.61 |
| ATOM | 1962 | CD1  | LEU | 208 | -37.280 | 27.460 | -5.994 | 1.00 | 17.00 |
| ATOM | 1963 | CD2  | LEU | 208 | -36.225 | 28.801 | -4.168 | 1.00 | 16.01 |
| ATOM | 1964 | H    | LEU | 208 | -32.833 | 27.711 | -6.326 | 1.00 | 0.00  |
| ATOM | 1965 | N    | GLN | 209 | -32.990 | 25.102 | -3.316 | 1.00 | 18.47 |
| ATOM | 1966 | CA   | GLN | 209 | -32.335 | 23.816 | -3.180 | 1.00 | 18.83 |
| ATOM | 1967 | C    | GLN | 209 | -33.379 | 22.802 | -3.609 | 1.00 | 18.98 |
| ATOM | 1968 | O    | GLN | 209 | -34.454 | 22.755 | -3.043 | 1.00 | 20.94 |
| ATOM | 1969 | CB   | GLN | 209 | -31.898 | 23.579 | -1.730 | 1.00 | 19.64 |
| ATOM | 1970 | CG   | GLN | 209 | -31.166 | 22.252 | -1.519 | 1.00 | 21.33 |
| ATOM | 1971 | CD   | GLN | 209 | -30.323 | 22.200 | -0.251 | 1.00 | 21.20 |
| ATOM | 1972 | OE1  | GLN | 209 | -29.552 | 21.261 | -0.055 | 1.00 | 21.45 |
| ATOM | 1973 | NE2  | GLN | 209 | -30.454 | 23.205 | 0.604  | 1.00 | 20.21 |
| ATOM | 1974 | H    | GLN | 209 | -33.435 | 25.549 | -2.566 | 1.00 | 0.00  |
| ATOM | 1975 | HE21 | GLN | 209 | -31.049 | 23.969 | 0.491  | 1.00 | 0.00  |
| ATOM | 1976 | HE22 | GLN | 209 | -29.865 | 23.056 | 1.378  | 1.00 | 0.00  |
| ATOM | 1977 | N    | ALA | 210 | -33.088 | 22.028 | -4.642 | 1.00 | 18.93 |
| ATOM | 1978 | CA   | ALA | 210 | -34.038 | 21.039 | -5.128 | 1.00 | 18.52 |
| ATOM | 1979 | C    | ALA | 210 | -33.884 | 19.710 | -4.412 | 1.00 | 18.46 |
| ATOM | 1980 | O    | ALA | 210 | -34.877 | 19.068 | -4.057 | 1.00 | 19.26 |
| ATOM | 1981 | CB   | ALA | 210 | -33.860 | 20.842 | -6.615 | 1.00 | 20.42 |
| ATOM | 1982 | H    | ALA | 210 | -32.212 | 22.074 | -5.068 | 1.00 | 0.00  |
| ATOM | 1983 | N    | GLY | 211 | -32.633 | 19.295 | -4.222 | 1.00 | 17.60 |
| ATOM | 1984 | CA   | GLY | 211 | -32.362 | 18.033 | -3.561 | 1.00 | 16.03 |
| ATOM | 1985 | C    | GLY | 211 | -31.060 | 17.966 | -2.783 | 1.00 | 15.45 |
| ATOM | 1986 | O    | GLY | 211 | -30.276 | 18.919 | -2.740 | 1.00 | 16.21 |
| ATOM | 1987 | H    | GLY | 211 | -31.891 | 19.864 | -4.517 | 1.00 | 0.00  |
| ATOM | 1988 | N    | VAL | 212 | -30.839 | 16.823 | -2.152 | 1.00 | 14.53 |
| ATOM | 1989 | CA   | VAL | 212 | -29.643 | 16.592 | -1.361 | 1.00 | 14.41 |
| ATOM | 1990 | C    | VAL | 212 | -28.975 | 15.321 | -1.895 | 1.00 | 14.88 |
| ATOM | 1991 | O    | VAL | 212 | -29.623 | 14.282 | -1.991 | 1.00 | 16.66 |
| ATOM | 1992 | CB   | VAL | 212 | -30.014 | 16.387 | 0.117  | 1.00 | 14.48 |
| ATOM | 1993 | CG1  | VAL | 212 | -28.775 | 16.243 | 0.956  | 1.00 | 16.33 |
| ATOM | 1994 | CG2  | VAL | 212 | -30.844 | 17.545 | 0.618  | 1.00 | 15.27 |
| ATOM | 1995 | H    | VAL | 212 | -31.525 | 16.129 | -2.211 | 1.00 | 0.00  |
| ATOM | 1996 | N    | VAL | 213 | -27.697 | 15.412 | -2.257 | 1.00 | 13.68 |

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|      |      |     |     |     |         |        |         |      |       |
|------|------|-----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1997 | CA  | VAL | 213 | -26.940 | 14.276 | -2.794  | 1.00 | 13.67 |
| ATOM | 1998 | C   | VAL | 213 | -27.112 | 12.999 | -1.967  | 1.00 | 15.32 |
| ATOM | 1999 | O   | VAL | 213 | -26.620 | 12.919 | -0.841  | 1.00 | 17.27 |
| ATOM | 2000 | CB  | VAL | 213 | -25.443 | 14.607 | -2.875  | 1.00 | 12.33 |
| ATOM | 2001 | CG1 | VAL | 213 | -24.684 | 13.445 | -3.477  | 1.00 | 11.91 |
| ATOM | 2002 | CG2 | VAL | 213 | -25.234 | 15.865 | -3.694  | 1.00 | 11.58 |
| ATOM | 2003 | H   | VAL | 213 | -27.280 | 16.294 | -2.134  | 1.00 | 0.00  |
| ATOM | 2004 | N   | SER | 214 | -27.759 | 11.991 | -2.549  | 1.00 | 15.85 |
| ATOM | 2005 | CA  | SER | 214 | -28.026 | 10.735 | -1.854  | 1.00 | 16.61 |
| ATOM | 2006 | C   | SER | 214 | -27.187 | 9.532  | -2.325  | 1.00 | 18.01 |
| ATOM | 2007 | O   | SER | 214 | -26.145 | 9.242  | -1.738  | 1.00 | 18.73 |
| ATOM | 2008 | CB  | SER | 214 | -29.531 | 10.435 | -1.921  | 1.00 | 15.37 |
| ATOM | 2009 | OG  | SER | 214 | -29.879 | 9.252  | -1.227  | 1.00 | 15.13 |
| ATOM | 2010 | H   | SER | 214 | -28.038 | 12.025 | -3.489  | 1.00 | 0.00  |
| ATOM | 2011 | HG  | SER | 214 | -29.747 | 9.329  | -0.267  | 1.00 | 0.00  |
| ATOM | 2012 | N   | TRP | 215 | -27.632 | 8.842  | -3.374  | 1.00 | 18.75 |
| ATOM | 2013 | CA  | TRP | 215 | -26.927 | 7.663  | -3.890  | 1.00 | 19.80 |
| ATOM | 2014 | C   | TRP | 215 | -26.723 | 7.645  | -5.414  | 1.00 | 22.23 |
| ATOM | 2015 | O   | TRP | 215 | -26.934 | 8.657  | -6.095  | 1.00 | 23.25 |
| ATOM | 2016 | CB  | TRP | 215 | -27.632 | 6.367  | -3.444  | 1.00 | 18.77 |
| ATOM | 2017 | CG  | TRP | 215 | -29.060 | 6.176  | -3.943  | 1.00 | 16.71 |
| ATOM | 2018 | CD1 | TRP | 215 | -30.158 | 6.912  | -3.592  | 1.00 | 16.79 |
| ATOM | 2019 | CD2 | TRP | 215 | -29.532 | 5.164  | -4.849  | 1.00 | 14.73 |
| ATOM | 2020 | NE1 | TRP | 215 | -31.275 | 6.420  | -4.217  | 1.00 | 16.69 |
| ATOM | 2021 | CE2 | TRP | 215 | -30.920 | 5.351  | -4.998  | 1.00 | 14.96 |
| ATOM | 2022 | CE3 | TRP | 215 | -28.914 | 4.114  | -5.543  | 1.00 | 15.88 |
| ATOM | 2023 | CZ2 | TRP | 215 | -31.709 | 4.525  | -5.820  | 1.00 | 14.57 |
| ATOM | 2024 | CZ3 | TRP | 215 | -29.701 | 3.290  | -6.360  | 1.00 | 14.45 |
| ATOM | 2025 | CH2 | TRP | 215 | -31.082 | 3.505  | -6.489  | 1.00 | 13.05 |
| ATOM | 2026 | H   | TRP | 215 | -28.431 | 9.140  | -3.848  | 1.00 | 0.00  |
| ATOM | 2027 | HE1 | TRP | 215 | -32.189 | 6.755  | -4.076  | 1.00 | 0.00  |
| ATOM | 2028 | N   | GLY | 216 | -26.297 | 6.494  | -5.931  | 1.00 | 22.70 |
| ATOM | 2029 | CA  | GLY | 216 | -26.056 | 6.339  | -7.355  | 1.00 | 24.31 |
| ATOM | 2030 | C   | GLY | 216 | -25.271 | 5.066  | -7.606  | 1.00 | 26.62 |
| ATOM | 2031 | O   | GLY | 216 | -24.638 | 4.555  | -6.683  | 1.00 | 26.51 |
| ATOM | 2032 | H   | GLY | 216 | -26.112 | 5.721  | -5.359  | 1.00 | 0.00  |
| ATOM | 2033 | N   | GLU | 217 | -25.357 | 4.523  | -8.817  | 1.00 | 28.89 |
| ATOM | 2034 | CA  | GLU | 217 | -24.637 | 3.301  | -9.169  | 1.00 | 30.51 |
| ATOM | 2035 | C   | GLU | 217 | -23.277 | 3.689  | -9.731  | 1.00 | 30.83 |
| ATOM | 2036 | O   | GLU | 217 | -22.945 | 3.327  | -10.856 | 1.00 | 32.11 |
| ATOM | 2037 | CB  | GLU | 217 | -25.403 | 2.517  | -10.240 | 1.00 | 33.50 |
| ATOM | 2038 | CG  | GLU | 217 | -26.856 | 2.197  | -9.906  | 1.00 | 37.89 |
| ATOM | 2039 | CD  | GLU | 217 | -27.040 | 0.848  | -9.240  | 1.00 | 39.20 |
| ATOM | 2040 | OE1 | GLU | 217 | -26.672 | 0.706  | -8.058  | 1.00 | 42.18 |
| ATOM | 2041 | OE2 | GLU | 217 | -27.578 | -0.077 | -9.881  | 1.00 | 38.06 |
| ATOM | 2042 | H   | GLU | 217 | -25.951 | 4.939  | -9.480  | 1.00 | 0.00  |
| ATOM | 2043 | N   | GLY | 219 | -22.491 | 4.417  | -8.942  | 1.00 | 30.52 |
| ATOM | 2044 | CA  | GLY | 219 | -21.183 | 4.864  | -9.393  | 1.00 | 29.85 |
| ATOM | 2045 | C   | GLY | 219 | -21.199 | 6.361  | -9.651  | 1.00 | 28.86 |
| ATOM | 2046 | O   | GLY | 219 | -22.056 | 7.067  | -9.125  | 1.00 | 29.70 |
| ATOM | 2047 | H   | GLY | 219 | -22.763 | 4.656  | -8.030  | 1.00 | 0.00  |
| ATOM | 2048 | N   | CYS | 220 | -20.255 | 6.849  | -10.445 | 1.00 | 27.30 |
| ATOM | 2049 | CA  | CYS | 220 | -20.183 | 8.270  | -10.765 | 1.00 | 26.59 |
| ATOM | 2050 | C   | CYS | 220 | -20.171 | 8.489  | -12.274 | 1.00 | 27.01 |
| ATOM | 2051 | O   | CYS | 220 | -19.342 | 7.921  | -12.978 | 1.00 | 27.63 |
| ATOM | 2052 | CB  | CYS | 220 | -18.931 | 8.895  | -10.145 | 1.00 | 25.63 |
| ATOM | 2053 | SG  | CYS | 220 | -18.899 | 8.829  | -8.329  | 1.00 | 24.76 |
| ATOM | 2054 | H   | CYS | 220 | -19.543 | 6.287  | -10.815 | 1.00 | 0.00  |
| ATOM | 2055 | N   | ALA | 221 | -21.101 | 9.302  | -12.763 | 1.00 | 27.64 |
| ATOM | 2056 | CA  | ALA | 221 | -21.218 | 9.622  | -14.184 | 1.00 | 27.24 |
| ATOM | 2057 | C   | ALA | 221 | -21.188 | 8.373  | -15.040 | 1.00 | 28.05 |
| ATOM | 2058 | O   | ALA | 221 | -20.558 | 8.339  | -16.099 | 1.00 | 29.91 |
| ATOM | 2059 | CB  | ALA | 221 | -20.119 | 10.579 | -14.606 | 1.00 | 27.26 |

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|      |      |      |     |      |         |        |         |      |       |
|------|------|------|-----|------|---------|--------|---------|------|-------|
| ATOM | 2060 | H    | ALA | 221  | -21.739 | 9.714  | -12.134 | 1.00 | 0.00  |
| ATOM | 2061 | N    | GLN | 221A | -21.853 | 7.332  | -14.563 | 1.00 | 28.12 |
| ATOM | 2062 | CA   | GLN | 221A | -21.904 | 6.086  | -15.297 | 1.00 | 27.89 |
| ATOM | 2063 | C    | GLN | 221A | -23.113 | 6.053  | -16.199 | 1.00 | 25.66 |
| ATOM | 2064 | O    | GLN | 221A | -24.199 | 6.472  | -15.811 | 1.00 | 26.52 |
| ATOM | 2065 | CB   | GLN | 221A | -21.945 | 4.900  | -14.347 | 1.00 | 30.43 |
| ATOM | 2066 | CG   | GLN | 221A | -20.590 | 4.309  | -14.085 | 1.00 | 34.17 |
| ATOM | 2067 | CD   | GLN | 221A | -20.683 | 3.020  | -13.314 | 1.00 | 38.53 |
| ATOM | 2068 | OE1  | GLN | 221A | -21.690 | 2.309  | -13.383 | 1.00 | 39.33 |
| ATOM | 2069 | NE2  | GLN | 221A | -19.632 | 2.703  | -12.566 | 1.00 | 41.61 |
| ATOM | 2070 | H    | GLN | 221A | -22.361 | 7.423  | -13.730 | 1.00 | 0.00  |
| ATOM | 2071 | HE21 | GLN | 221A | -18.875 | 3.322  | -12.536 | 1.00 | 0.00  |
| ATOM | 2072 | HE22 | GLN | 221A | -19.692 | 1.857  | -12.082 | 1.00 | 0.00  |
| ATOM | 2073 | N    | PRO | 222  | -22.940 | 5.546  | -17.418 | 1.00 | 23.92 |
| ATOM | 2074 | CA   | PRO | 222  | -23.998 | 5.434  | -18.418 | 1.00 | 24.23 |
| ATOM | 2075 | C    | PRO | 222  | -25.267 | 4.778  | -17.866 | 1.00 | 24.53 |
| ATOM | 2076 | O    | PRO | 222  | -25.214 | 3.679  | -17.318 | 1.00 | 25.97 |
| ATOM | 2077 | CB   | PRO | 222  | -23.351 | 4.544  | -19.473 | 1.00 | 24.60 |
| ATOM | 2078 | CG   | PRO | 222  | -21.927 | 4.947  | -19.403 | 1.00 | 25.12 |
| ATOM | 2079 | CD   | PRO | 222  | -21.678 | 4.992  | -17.930 | 1.00 | 24.30 |
| ATOM | 2080 | N    | ASN | 223  | -26.395 | 5.466  | -18.019 | 1.00 | 24.28 |
| ATOM | 2081 | CA   | ASN | 223  | -27.709 | 4.993  | -17.581 | 1.00 | 24.70 |
| ATOM | 2082 | C    | ASN | 223  | -27.979 | 4.903  | -16.091 | 1.00 | 24.56 |
| ATOM | 2083 | O    | ASN | 223  | -28.965 | 4.291  | -15.667 | 1.00 | 26.39 |
| ATOM | 2084 | CB   | ASN | 223  | -28.058 | 3.669  | -18.248 | 1.00 | 26.24 |
| ATOM | 2085 | CG   | ASN | 223  | -28.585 | 3.853  | -19.644 | 1.00 | 27.52 |
| ATOM | 2086 | OD1  | ASN | 223  | -29.115 | 4.916  | -19.989 | 1.00 | 29.20 |
| ATOM | 2087 | ND2  | ASN | 223  | -28.464 | 2.822  | -20.457 | 1.00 | 28.84 |
| ATOM | 2088 | H    | ASN | 223  | -26.346 | 6.344  | -18.442 | 1.00 | 0.00  |
| ATOM | 2089 | HD21 | ASN | 223  | -28.045 | 2.016  | -20.087 | 1.00 | 0.00  |
| ATOM | 2090 | HD22 | ASN | 223  | -28.780 | 2.888  | -21.377 | 1.00 | 0.00  |
| ATOM | 2091 | N    | ARG | 224  | -27.109 | 5.504  | -15.296 | 1.00 | 22.65 |
| ATOM | 2092 | CA   | ARG | 224  | -27.271 | 5.508  | -13.854 | 1.00 | 21.59 |
| ATOM | 2093 | C    | ARG | 224  | -27.132 | 6.954  | -13.403 | 1.00 | 21.52 |
| ATOM | 2094 | O    | ARG | 224  | -26.072 | 7.366  | -12.923 | 1.00 | 23.00 |
| ATOM | 2095 | CB   | ARG | 224  | -26.183 | 4.653  | -13.209 | 1.00 | 21.30 |
| ATOM | 2096 | CG   | ARG | 224  | -26.100 | 3.248  | -13.767 | 1.00 | 20.28 |
| ATOM | 2097 | CD   | ARG | 224  | -27.446 | 2.572  | -13.710 | 1.00 | 17.59 |
| ATOM | 2098 | NE   | ARG | 224  | -27.359 | 1.149  | -13.986 | 1.00 | 14.62 |
| ATOM | 2099 | CZ   | ARG | 224  | -28.133 | 0.513  | -14.857 | 1.00 | 14.61 |
| ATOM | 2100 | NH1  | ARG | 224  | -29.043 | 1.188  | -15.557 | 1.00 | 13.22 |
| ATOM | 2101 | NH2  | ARG | 224  | -28.042 | -0.808 | -14.972 | 1.00 | 13.90 |
| ATOM | 2102 | H    | ARG | 224  | -26.287 | 5.922  | -15.626 | 1.00 | 0.00  |
| ATOM | 2103 | HE   | ARG | 224  | -26.664 | 0.657  | -13.479 | 1.00 | 0.00  |
| ATOM | 2104 | HH11 | ARG | 224  | -29.184 | 2.177  | -15.478 | 1.00 | 0.00  |
| ATOM | 2105 | HH12 | ARG | 224  | -29.625 | 0.692  | -16.207 | 1.00 | 0.00  |
| ATOM | 2106 | HH21 | ARG | 224  | -27.488 | -1.374 | -14.351 | 1.00 | 0.00  |
| ATOM | 2107 | HH22 | ARG | 224  | -28.666 | -1.283 | -15.586 | 1.00 | 0.00  |
| ATOM | 2108 | N    | PRO | 225  | -28.177 | 7.764  | -13.619 | 1.00 | 20.05 |
| ATOM | 2109 | CA   | PRO | 225  | -28.142 | 9.176  | -13.225 | 1.00 | 19.00 |
| ATOM | 2110 | C    | PRO | 225  | -27.960 | 9.334  | -11.710 | 1.00 | 18.85 |
| ATOM | 2111 | O    | PRO | 225  | -28.180 | 8.381  | -10.947 | 1.00 | 18.87 |
| ATOM | 2112 | CB   | PRO | 225  | -29.508 | 9.690  | -13.680 | 1.00 | 19.40 |
| ATOM | 2113 | CG   | PRO | 225  | -29.894 | 8.742  | -14.788 | 1.00 | 19.39 |
| ATOM | 2114 | CD   | PRO | 225  | -29.463 | 7.423  | -14.247 | 1.00 | 19.45 |
| ATOM | 2115 | N    | GLY | 226  | -27.561 | 10.528 | -11.279 | 1.00 | 16.97 |
| ATOM | 2116 | CA   | GLY | 226  | -27.362 | 10.767 | -9.864  | 1.00 | 14.75 |
| ATOM | 2117 | C    | GLY | 226  | -28.711 | 10.884 | -9.195  | 1.00 | 14.13 |
| ATOM | 2118 | O    | GLY | 226  | -29.627 | 11.488 | -9.766  | 1.00 | 14.36 |
| ATOM | 2119 | H    | GLY | 226  | -27.436 | 11.301 | -11.865 | 1.00 | 0.00  |
| ATOM | 2120 | N    | ILE | 227  | -28.862 | 10.272 | -8.022  | 1.00 | 13.51 |
| ATOM | 2121 | CA   | ILE | 227  | -30.122 | 10.338 | -7.288  | 1.00 | 11.82 |
| ATOM | 2122 | C    | ILE | 227  | -29.941 | 11.290 | -6.117  | 1.00 | 12.42 |

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|      |      |      |     |     |         |        |         |      |       |
|------|------|------|-----|-----|---------|--------|---------|------|-------|
| ATOM | 2123 | O    | ILE | 227 | -28.919 | 11.265 | -5.431  | 1.00 | 12.50 |
| ATOM | 2124 | CB   | ILE | 227 | -30.564 | 8.970  | -6.754  | 1.00 | 10.14 |
| ATOM | 2125 | CG1  | ILE | 227 | -30.491 | 7.914  | -7.863  | 1.00 | 10.02 |
| ATOM | 2126 | CG2  | ILE | 227 | -31.961 | 9.070  | -6.162  | 1.00 | 8.00  |
| ATOM | 2127 | H    | ILE | 227 | -28.129 | 9.777  | -7.603  | 1.00 | 0.00  |
| ATOM | 2128 | CD   | ILE | 227 | -31.155 | 8.318  | -9.162  | 1.00 | 10.22 |
| ATOM | 2129 | N    | TYR | 228 | -30.911 | 12.171 | -5.934  | 1.00 | 12.70 |
| ATOM | 2130 | CA   | TYR | 228 | -30.877 | 13.153 | -4.865  | 1.00 | 14.33 |
| ATOM | 2131 | C    | TYR | 228 | -32.193 | 13.052 | -4.106  | 1.00 | 15.62 |
| ATOM | 2132 | O    | TYR | 228 | -33.197 | 12.609 | -4.652  | 1.00 | 17.70 |
| ATOM | 2133 | CB   | TYR | 228 | -30.737 | 14.571 | -5.445  | 1.00 | 14.73 |
| ATOM | 2134 | CG   | TYR | 228 | -29.502 | 14.806 | -6.295  | 1.00 | 14.85 |
| ATOM | 2135 | CD1  | TYR | 228 | -29.272 | 14.055 | -7.443  | 1.00 | 16.42 |
| ATOM | 2136 | CD2  | TYR | 228 | -28.556 | 15.764 | -5.940  | 1.00 | 14.70 |
| ATOM | 2137 | CE1  | TYR | 228 | -28.130 | 14.241 | -8.214  | 1.00 | 17.69 |
| ATOM | 2138 | CE2  | TYR | 228 | -27.410 | 15.961 | -6.706  | 1.00 | 15.13 |
| ATOM | 2139 | CZ   | TYR | 228 | -27.203 | 15.192 | -7.840  | 1.00 | 16.67 |
| ATOM | 2140 | OH   | TYR | 228 | -26.062 | 15.334 | -8.593  | 1.00 | 17.66 |
| ATOM | 2141 | H    | TYR | 228 | -31.654 | 12.164 | -6.559  | 1.00 | 0.00  |
| ATOM | 2142 | HH   | TYR | 228 | -25.499 | 15.977 | -8.168  | 1.00 | 0.00  |
| ATOM | 2143 | N    | THR | 229 | -32.176 | 13.430 | -2.837  | 1.00 | 14.78 |
| ATOM | 2144 | CA   | THR | 229 | -33.374 | 13.401 | -2.032  | 1.00 | 14.18 |
| ATOM | 2145 | C    | THR | 229 | -34.163 | 14.617 | -2.457  | 1.00 | 15.59 |
| ATOM | 2146 | O    | THR | 229 | -33.646 | 15.735 | -2.408  | 1.00 | 16.40 |
| ATOM | 2147 | CB   | THR | 229 | -33.037 | 13.540 | -0.556  | 1.00 | 13.98 |
| ATOM | 2148 | OG1  | THR | 229 | -31.932 | 12.688 | -0.249  | 1.00 | 15.24 |
| ATOM | 2149 | CG2  | THR | 229 | -34.221 | 13.126 | 0.294   | 1.00 | 15.09 |
| ATOM | 2150 | H    | THR | 229 | -31.335 | 13.707 | -2.436  | 1.00 | 0.00  |
| ATOM | 2151 | HG1  | THR | 229 | -31.083 | 13.131 | -0.319  | 1.00 | 0.00  |
| ATOM | 2152 | N    | ARG | 230 | -35.398 | 14.400 | -2.896  | 1.00 | 16.90 |
| ATOM | 2153 | CA   | ARG | 230 | -36.256 | 15.492 | -3.337  | 1.00 | 18.50 |
| ATOM | 2154 | C    | ARG | 230 | -36.680 | 16.284 | -2.104  | 1.00 | 20.13 |
| ATOM | 2155 | O    | ARG | 230 | -37.521 | 15.833 | -1.326  | 1.00 | 21.66 |
| ATOM | 2156 | CB   | ARG | 230 | -37.474 | 14.938 | -4.074  | 1.00 | 17.41 |
| ATOM | 2157 | CG   | ARG | 230 | -38.252 | 15.981 | -4.833  | 1.00 | 18.25 |
| ATOM | 2158 | CD   | ARG | 230 | -39.242 | 15.349 | -5.791  | 1.00 | 19.18 |
| ATOM | 2159 | NE   | ARG | 230 | -39.194 | 16.003 | -7.096  | 1.00 | 20.74 |
| ATOM | 2160 | CZ   | ARG | 230 | -38.796 | 15.398 | -8.208  | 1.00 | 22.85 |
| ATOM | 2161 | NH1  | ARG | 230 | -38.425 | 14.124 | -8.168  | 1.00 | 24.02 |
| ATOM | 2162 | NH2  | ARG | 230 | -38.699 | 16.082 | -9.340  | 1.00 | 24.49 |
| ATOM | 2163 | H    | ARG | 230 | -35.770 | 13.496 | -2.857  | 1.00 | 0.00  |
| ATOM | 2164 | HE   | ARG | 230 | -39.467 | 16.949 | -7.119  | 1.00 | 0.00  |
| ATOM | 2165 | HH11 | ARG | 230 | -38.419 | 13.561 | -7.330  | 1.00 | 0.00  |
| ATOM | 2166 | HH12 | ARG | 230 | -38.147 | 13.602 | -8.987  | 1.00 | 0.00  |
| ATOM | 2167 | HH21 | ARG | 230 | -38.897 | 17.070 | -9.444  | 1.00 | 0.00  |
| ATOM | 2168 | HH22 | ARG | 230 | -38.385 | 15.644 | -10.188 | 1.00 | 0.00  |
| ATOM | 2169 | N    | VAL | 231 | -36.106 | 17.473 | -1.944  | 1.00 | 20.07 |
| ATOM | 2170 | CA   | VAL | 231 | -36.383 | 18.318 | -0.795  | 1.00 | 19.37 |
| ATOM | 2171 | C    | VAL | 231 | -37.842 | 18.701 | -0.567  | 1.00 | 20.92 |
| ATOM | 2172 | O    | VAL | 231 | -38.301 | 18.664 | 0.570   | 1.00 | 22.84 |
| ATOM | 2173 | CB   | VAL | 231 | -35.485 | 19.562 | -0.798  | 1.00 | 18.36 |
| ATOM | 2174 | CG1  | VAL | 231 | -35.830 | 20.484 | 0.352   | 1.00 | 17.59 |
| ATOM | 2175 | CG2  | VAL | 231 | -34.046 | 19.133 | -0.679  | 1.00 | 18.89 |
| ATOM | 2176 | H    | VAL | 231 | -35.526 | 17.822 | -2.653  | 1.00 | 0.00  |
| ATOM | 2177 | N    | THR | 232 | -38.592 | 19.032 | -1.618  | 1.00 | 22.13 |
| ATOM | 2178 | CA   | THR | 232 | -40.003 | 19.406 | -1.428  | 1.00 | 22.78 |
| ATOM | 2179 | C    | THR | 232 | -40.817 | 18.329 | -0.692  | 1.00 | 21.93 |
| ATOM | 2180 | O    | THR | 232 | -41.702 | 18.649 | 0.104   | 1.00 | 21.21 |
| ATOM | 2181 | CB   | THR | 232 | -40.718 | 19.806 | -2.773  | 1.00 | 23.61 |
| ATOM | 2182 | OG1  | THR | 232 | -40.517 | 18.797 | -3.775  | 1.00 | 24.69 |
| ATOM | 2183 | CG2  | THR | 232 | -40.202 | 21.145 | -3.289  | 1.00 | 23.76 |
| ATOM | 2184 | H    | THR | 232 | -38.233 | 19.038 | -2.526  | 1.00 | 0.00  |
| ATOM | 2185 | HG1  | THR | 232 | -40.723 | 19.294 | -4.589  | 1.00 | 0.00  |

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|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 2186 | N   | TYR | 233 | -40.430 | 17.068 | -0.885 | 1.00 | 22.13 |
| ATOM | 2187 | CA  | TYR | 233 | -41.100 | 15.905 | -0.285 | 1.00 | 21.64 |
| ATOM | 2188 | C   | TYR | 233 | -41.059 | 15.890 | 1.248  | 1.00 | 22.23 |
| ATOM | 2189 | O   | TYR | 233 | -41.997 | 15.414 | 1.900  | 1.00 | 23.30 |
| ATOM | 2190 | CB  | TYR | 233 | -40.461 | 14.620 | -0.830 | 1.00 | 20.12 |
| ATOM | 2191 | CG  | TYR | 233 | -41.255 | 13.345 | -0.639 | 1.00 | 20.42 |
| ATOM | 2192 | CD1 | TYR | 233 | -41.793 | 12.670 | -1.730 | 1.00 | 20.53 |
| ATOM | 2193 | CD2 | TYR | 233 | -41.417 | 12.778 | 0.620  | 1.00 | 21.24 |
| ATOM | 2194 | CE1 | TYR | 233 | -42.467 | 11.462 | -1.573 | 1.00 | 20.50 |
| ATOM | 2195 | CE2 | TYR | 233 | -42.089 | 11.574 | 0.789  | 1.00 | 21.23 |
| ATOM | 2196 | CZ  | TYR | 233 | -42.610 | 10.920 | -0.312 | 1.00 | 21.44 |
| ATOM | 2197 | OH  | TYR | 233 | -43.272 | 9.726  | -0.134 | 1.00 | 23.83 |
| ATOM | 2198 | H   | TYR | 233 | -39.636 | 16.905 | -1.431 | 1.00 | 0.00  |
| ATOM | 2199 | HH  | TYR | 233 | -43.635 | 9.360  | -0.962 | 1.00 | 0.00  |
| ATOM | 2200 | N   | TYR | 234 | -39.980 | 16.423 | 1.816  | 1.00 | 21.17 |
| ATOM | 2201 | CA  | TYR | 234 | -39.799 | 16.448 | 3.262  | 1.00 | 18.57 |
| ATOM | 2202 | C   | TYR | 234 | -39.844 | 17.850 | 3.846  | 1.00 | 19.36 |
| ATOM | 2203 | O   | TYR | 234 | -39.351 | 18.073 | 4.951  | 1.00 | 20.52 |
| ATOM | 2204 | CB  | TYR | 234 | -38.465 | 15.791 | 3.623  | 1.00 | 15.70 |
| ATOM | 2205 | CG  | TYR | 234 | -38.396 | 14.343 | 3.226  | 1.00 | 13.09 |
| ATOM | 2206 | CD1 | TYR | 234 | -37.601 | 13.921 | 2.162  | 1.00 | 10.69 |
| ATOM | 2207 | CD2 | TYR | 234 | -39.173 | 13.398 | 3.885  | 1.00 | 13.26 |
| ATOM | 2208 | CE1 | TYR | 234 | -37.593 | 12.592 | 1.763  | 1.00 | 9.73  |
| ATOM | 2209 | CE2 | TYR | 234 | -39.172 | 12.067 | 3.495  | 1.00 | 12.18 |
| ATOM | 2210 | CZ  | TYR | 234 | -38.386 | 11.670 | 2.436  | 1.00 | 11.33 |
| ATOM | 2211 | OH  | TYR | 234 | -38.415 | 10.349 | 2.053  | 1.00 | 12.19 |
| ATOM | 2212 | H   | TYR | 234 | -39.296 | 16.846 | 1.255  | 1.00 | 0.00  |
| ATOM | 2213 | HH  | TYR | 234 | -39.230 | 9.921  | 2.315  | 1.00 | 0.00  |
| ATOM | 2214 | N   | LEU | 235 | -40.484 | 18.777 | 3.146  | 1.00 | 19.94 |
| ATOM | 2215 | CA  | LEU | 235 | -40.556 | 20.150 | 3.622  | 1.00 | 22.71 |
| ATOM | 2216 | C   | LEU | 235 | -41.166 | 20.337 | 5.004  | 1.00 | 26.74 |
| ATOM | 2217 | O   | LEU | 235 | -40.578 | 21.015 | 5.846  | 1.00 | 28.36 |
| ATOM | 2218 | CB  | LEU | 235 | -41.278 | 21.039 | 2.616  | 1.00 | 21.13 |
| ATOM | 2219 | CG  | LEU | 235 | -40.398 | 21.688 | 1.551  | 1.00 | 19.17 |
| ATOM | 2220 | CD1 | LEU | 235 | -41.288 | 22.370 | 0.542  | 1.00 | 17.42 |
| ATOM | 2221 | CD2 | LEU | 235 | -39.429 | 22.671 | 2.185  | 1.00 | 16.49 |
| ATOM | 2222 | H   | LEU | 235 | -40.918 | 18.542 | 2.295  | 1.00 | 0.00  |
| ATOM | 2223 | N   | ASP | 236 | -42.336 | 19.755 | 5.250  | 1.00 | 30.41 |
| ATOM | 2224 | CA  | ASP | 236 | -42.978 | 19.910 | 6.555  | 1.00 | 33.46 |
| ATOM | 2225 | C   | ASP | 236 | -42.112 | 19.336 | 7.667  | 1.00 | 31.07 |
| ATOM | 2226 | O   | ASP | 236 | -41.904 | 19.980 | 8.695  | 1.00 | 32.26 |
| ATOM | 2227 | CB  | ASP | 236 | -44.369 | 19.266 | 6.576  | 1.00 | 40.96 |
| ATOM | 2228 | CG  | ASP | 236 | -45.112 | 19.504 | 7.902  | 1.00 | 47.92 |
| ATOM | 2229 | OD1 | ASP | 236 | -45.024 | 20.624 | 8.470  | 1.00 | 49.63 |
| ATOM | 2230 | OD2 | ASP | 236 | -45.780 | 18.556 | 8.385  | 1.00 | 51.27 |
| ATOM | 2231 | H   | ASP | 236 | -42.779 | 19.227 | 4.561  | 1.00 | 0.00  |
| ATOM | 2232 | N   | TRP | 237 | -41.583 | 18.138 | 7.446  | 1.00 | 27.60 |
| ATOM | 2233 | CA  | TRP | 237 | -40.718 | 17.495 | 8.427  | 1.00 | 25.41 |
| ATOM | 2234 | C   | TRP | 237 | -39.588 | 18.466 | 8.783  | 1.00 | 26.42 |
| ATOM | 2235 | O   | TRP | 237 | -39.330 | 18.735 | 9.964  | 1.00 | 25.41 |
| ATOM | 2236 | CB  | TRP | 237 | -40.150 | 16.194 | 7.857  | 1.00 | 22.16 |
| ATOM | 2237 | CG  | TRP | 237 | -39.293 | 15.454 | 8.822  | 1.00 | 18.39 |
| ATOM | 2238 | CD1 | TRP | 237 | -39.711 | 14.640 | 9.831  | 1.00 | 18.35 |
| ATOM | 2239 | CD2 | TRP | 237 | -37.870 | 15.495 | 8.901  | 1.00 | 15.74 |
| ATOM | 2240 | NE1 | TRP | 237 | -38.632 | 14.179 | 10.542 | 1.00 | 16.42 |
| ATOM | 2241 | CE2 | TRP | 237 | -37.489 | 14.687 | 9.991  | 1.00 | 15.10 |
| ATOM | 2242 | CE3 | TRP | 237 | -36.879 | 16.141 | 8.157  | 1.00 | 14.45 |
| ATOM | 2243 | CZ2 | TRP | 237 | -36.161 | 14.504 | 10.356 | 1.00 | 15.23 |
| ATOM | 2244 | CZ3 | TRP | 237 | -35.561 | 15.962 | 8.520  | 1.00 | 14.94 |
| ATOM | 2245 | CH2 | TRP | 237 | -35.211 | 15.149 | 9.612  | 1.00 | 15.76 |
| ATOM | 2246 | H   | TRP | 237 | -41.807 | 17.685 | 6.611  | 1.00 | 0.00  |
| ATOM | 2247 | HE1 | TRP | 237 | -38.689 | 13.658 | 11.374 | 1.00 | 0.00  |
| ATOM | 2248 | N   | ILE | 238 | -38.947 | 19.011 | 7.751  | 1.00 | 27.11 |

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|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 2249 | CA  | ILE | 238 | -37.871 | 19.979 | 7.928  | 1.00 | 27.21 |
| ATOM | 2250 | C   | ILE | 238 | -38.415 | 21.102 | 8.792  | 1.00 | 28.94 |
| ATOM | 2251 | O   | ILE | 238 | -37.873 | 21.403 | 9.849  | 1.00 | 29.26 |
| ATOM | 2252 | CB  | ILE | 238 | -37.422 | 20.588 | 6.569  | 1.00 | 24.63 |
| ATOM | 2253 | CG1 | ILE | 238 | -36.730 | 19.531 | 5.710  | 1.00 | 23.19 |
| ATOM | 2254 | CG2 | ILE | 238 | -36.499 | 21.765 | 6.796  | 1.00 | 23.54 |
| ATOM | 2255 | H   | ILE | 238 | -39.168 | 18.732 | 6.837  | 1.00 | 0.00  |
| ATOM | 2256 | CD  | ILE | 238 | -36.514 | 19.951 | 4.282  | 1.00 | 20.94 |
| ATOM | 2257 | N   | HIS | 239 | -39.539 | 21.667 | 8.367  | 1.00 | 31.87 |
| ATOM | 2258 | CA  | HIS | 239 | -40.155 | 22.770 | 9.084  | 1.00 | 36.00 |
| ATOM | 2259 | C   | HIS | 239 | -40.585 | 22.451 | 10.499 | 1.00 | 38.31 |
| ATOM | 2260 | O   | HIS | 239 | -40.769 | 23.355 | 11.308 | 1.00 | 39.77 |
| ATOM | 2261 | CB  | HIS | 239 | -41.292 | 23.388 | 8.267  | 1.00 | 37.85 |
| ATOM | 2262 | CG  | HIS | 239 | -40.805 | 24.234 | 7.130  | 1.00 | 41.11 |
| ATOM | 2263 | ND1 | HIS | 239 | -39.756 | 25.122 | 7.263  | 1.00 | 42.70 |
| ATOM | 2264 | CD2 | HIS | 239 | -41.179 | 24.290 | 5.829  | 1.00 | 42.19 |
| ATOM | 2265 | CE1 | HIS | 239 | -39.498 | 25.681 | 6.094  | 1.00 | 42.65 |
| ATOM | 2266 | NE2 | HIS | 239 | -40.347 | 25.194 | 5.207  | 1.00 | 44.13 |
| ATOM | 2267 | H   | HIS | 239 | -39.954 | 21.331 | 7.554  | 1.00 | 0.00  |
| ATOM | 2268 | HD1 | HIS | 239 | -39.283 | 25.298 | 8.117  | 1.00 | 0.00  |
| ATOM | 2269 | HE2 | HIS | 239 | -40.372 | 25.429 | 4.254  | 1.00 | 0.00  |
| ATOM | 2270 | N   | HIS | 240 | -40.698 | 21.169 | 10.817 | 1.00 | 40.57 |
| ATOM | 2271 | CA  | HIS | 240 | -41.071 | 20.772 | 12.165 | 1.00 | 43.12 |
| ATOM | 2272 | C   | HIS | 240 | -39.976 | 21.199 | 13.120 | 1.00 | 42.47 |
| ATOM | 2273 | O   | HIS | 240 | -40.231 | 21.476 | 14.289 | 1.00 | 42.87 |
| ATOM | 2274 | CB  | HIS | 240 | -41.245 | 19.257 | 12.259 | 1.00 | 48.45 |
| ATOM | 2275 | CG  | HIS | 240 | -42.552 | 18.765 | 11.727 | 1.00 | 54.77 |
| ATOM | 2276 | ND1 | HIS | 240 | -42.921 | 17.436 | 11.764 | 1.00 | 57.09 |
| ATOM | 2277 | CD2 | HIS | 240 | -43.589 | 19.427 | 11.159 | 1.00 | 57.17 |
| ATOM | 2278 | CE1 | HIS | 240 | -44.128 | 17.302 | 11.241 | 1.00 | 59.02 |
| ATOM | 2279 | NE2 | HIS | 240 | -44.554 | 18.495 | 10.866 | 1.00 | 59.61 |
| ATOM | 2280 | H   | HIS | 240 | -40.560 | 20.499 | 10.115 | 1.00 | 0.00  |
| ATOM | 2281 | HD1 | HIS | 240 | -42.372 | 16.697 | 12.103 | 1.00 | 0.00  |
| ATOM | 2282 | HE2 | HIS | 240 | -45.367 | 18.707 | 10.332 | 1.00 | 0.00  |
| ATOM | 2283 | N   | TYR | 241 | -38.757 | 21.261 | 12.600 | 1.00 | 41.62 |
| ATOM | 2284 | CA  | TYR | 241 | -37.598 | 21.621 | 13.394 | 1.00 | 39.89 |
| ATOM | 2285 | C   | TYR | 241 | -37.064 | 22.995 | 13.033 | 1.00 | 40.78 |
| ATOM | 2286 | O   | TYR | 241 | -36.720 | 23.785 | 13.912 | 1.00 | 41.42 |
| ATOM | 2287 | CB  | TYR | 241 | -36.518 | 20.556 | 13.209 | 1.00 | 37.39 |
| ATOM | 2288 | CG  | TYR | 241 | -37.006 | 19.162 | 13.548 | 1.00 | 35.05 |
| ATOM | 2289 | CD1 | TYR | 241 | -37.460 | 18.292 | 12.555 | 1.00 | 33.81 |
| ATOM | 2290 | CD2 | TYR | 241 | -37.043 | 18.725 | 14.870 | 1.00 | 34.80 |
| ATOM | 2291 | CE1 | TYR | 241 | -37.940 | 17.023 | 12.878 | 1.00 | 33.34 |
| ATOM | 2292 | CE2 | TYR | 241 | -37.518 | 17.463 | 15.204 | 1.00 | 33.45 |
| ATOM | 2293 | CZ  | TYR | 241 | -37.966 | 16.619 | 14.210 | 1.00 | 33.44 |
| ATOM | 2294 | OH  | TYR | 241 | -38.434 | 15.373 | 14.565 | 1.00 | 32.52 |
| ATOM | 2295 | H   | TYR | 241 | -38.620 | 21.061 | 11.652 | 1.00 | 0.00  |
| ATOM | 2296 | HH  | TYR | 241 | -38.322 | 15.249 | 15.506 | 1.00 | 0.00  |
| ATOM | 2297 | N   | VAL | 242 | -37.011 | 23.285 | 11.740 | 1.00 | 42.12 |
| ATOM | 2298 | CA  | VAL | 242 | -36.508 | 24.565 | 11.265 | 1.00 | 43.92 |
| ATOM | 2299 | C   | VAL | 242 | -37.606 | 25.618 | 11.126 | 1.00 | 46.59 |
| ATOM | 2300 | O   | VAL | 242 | -38.502 | 25.496 | 10.285 | 1.00 | 46.87 |
| ATOM | 2301 | CB  | VAL | 242 | -35.762 | 24.409 | 9.921  | 1.00 | 43.14 |
| ATOM | 2302 | CG1 | VAL | 242 | -35.229 | 25.750 | 9.454  | 1.00 | 42.99 |
| ATOM | 2303 | CG2 | VAL | 242 | -34.627 | 23.409 | 10.067 | 1.00 | 42.58 |
| ATOM | 2304 | H   | VAL | 242 | -37.315 | 22.619 | 11.101 | 1.00 | 0.00  |
| ATOM | 2305 | N   | PRO | 243 | -37.528 | 26.688 | 11.932 | 1.00 | 48.74 |
| ATOM | 2306 | CA  | PRO | 243 | -38.508 | 27.775 | 11.910 | 1.00 | 51.59 |
| ATOM | 2307 | C   | PRO | 243 | -38.460 | 28.613 | 10.637 | 1.00 | 54.17 |
| ATOM | 2308 | O   | PRO | 243 | -37.439 | 28.671 | 9.950  | 1.00 | 54.00 |
| ATOM | 2309 | CB  | PRO | 243 | -38.100 | 28.611 | 13.123 | 1.00 | 50.78 |
| ATOM | 2310 | CG  | PRO | 243 | -36.616 | 28.423 | 13.176 | 1.00 | 48.29 |
| ATOM | 2311 | CD  | PRO | 243 | -36.502 | 26.937 | 12.961 | 1.00 | 49.12 |

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 2312 | N   | LYS | 244 | -39.571 | 29.275 | 10.344 | 1.00 | 58.19 |
| ATOM | 2313 | CA  | LYS | 244 | -39.673 | 30.146 | 9.179  | 1.00 | 63.13 |
| ATOM | 2314 | C   | LYS | 244 | -38.702 | 31.323 | 9.336  | 1.00 | 65.28 |
| ATOM | 2315 | O   | LYS | 244 | -38.832 | 32.130 | 10.271 | 1.00 | 65.32 |
| ATOM | 2316 | CB  | LYS | 244 | -41.104 | 30.685 | 9.058  | 1.00 | 65.63 |
| ATOM | 2317 | CG  | LYS | 244 | -41.311 | 31.701 | 7.932  | 1.00 | 68.20 |
| ATOM | 2318 | CD  | LYS | 244 | -42.362 | 32.763 | 8.288  | 1.00 | 69.17 |
| ATOM | 2319 | CE  | LYS | 244 | -41.848 | 33.732 | 9.354  | 1.00 | 70.12 |
| ATOM | 2320 | NZ  | LYS | 244 | -42.789 | 34.862 | 9.619  | 1.00 | 70.75 |
| ATOM | 2321 | H   | LYS | 244 | -40.346 | 29.153 | 10.929 | 1.00 | 0.00  |
| ATOM | 2322 | HZ1 | LYS | 244 | -43.698 | 34.486 | 9.956  | 1.00 | 0.00  |
| ATOM | 2323 | HZ2 | LYS | 244 | -42.930 | 35.415 | 8.753  | 1.00 | 0.00  |
| ATOM | 2324 | HZ3 | LYS | 244 | -42.389 | 35.478 | 10.355 | 1.00 | 0.00  |
| ATOM | 2325 | N   | LYS | 245 | -37.733 | 31.424 | 8.427  | 1.00 | 67.30 |
| ATOM | 2326 | CA  | LYS | 245 | -36.752 | 32.509 | 8.467  | 1.00 | 68.35 |
| ATOM | 2327 | C   | LYS | 245 | -35.876 | 32.535 | 7.213  | 1.00 | 68.88 |
| ATOM | 2328 | O   | LYS | 245 | -34.838 | 31.869 | 7.147  | 1.00 | 69.36 |
| ATOM | 2329 | CB  | LYS | 245 | -35.879 | 32.384 | 9.720  | 1.00 | 68.59 |
| ATOM | 2330 | CG  | LYS | 245 | -35.528 | 33.711 | 10.356 | 1.00 | 68.95 |
| ATOM | 2331 | CD  | LYS | 245 | -35.187 | 33.544 | 11.829 | 1.00 | 69.64 |
| ATOM | 2332 | CE  | LYS | 245 | -36.318 | 32.866 | 12.608 | 1.00 | 70.40 |
| ATOM | 2333 | NZ  | LYS | 245 | -37.664 | 33.481 | 12.387 | 1.00 | 70.71 |
| ATOM | 2334 | H   | LYS | 245 | -37.652 | 30.738 | 7.725  | 1.00 | 0.00  |
| ATOM | 2335 | HZ1 | LYS | 245 | -38.007 | 33.241 | 11.430 | 1.00 | 0.00  |
| ATOM | 2336 | HZ2 | LYS | 245 | -37.641 | 34.506 | 12.545 | 1.00 | 0.00  |
| ATOM | 2337 | HZ3 | LYS | 245 | -38.337 | 33.047 | 13.048 | 1.00 | 0.00  |
| TER  | 2338 |     | LYS | 245 |         |        |        |      |       |
| ATOM | 2339 | N   | ILE | 16  | 8.303   | 15.213 | 9.545  | 1.00 | 19.59 |
| ATOM | 2340 | CA  | ILE | 16  | 9.155   | 15.357 | 10.715 | 1.00 | 19.19 |
| ATOM | 2341 | C   | ILE | 16  | 8.537   | 14.666 | 11.932 | 1.00 | 20.42 |
| ATOM | 2342 | O   | ILE | 16  | 7.401   | 14.970 | 12.326 | 1.00 | 20.07 |
| ATOM | 2343 | CB  | ILE | 16  | 9.384   | 16.846 | 11.047 | 1.00 | 18.18 |
| ATOM | 2344 | CG1 | ILE | 16  | 10.152  | 17.536 | 9.918  | 1.00 | 18.36 |
| ATOM | 2345 | CG2 | ILE | 16  | 10.108  | 16.991 | 12.368 | 1.00 | 18.50 |
| ATOM | 2346 | H   | ILE | 16  | 8.210   | 14.319 | 9.140  | 1.00 | 0.00  |
| ATOM | 2347 | CD  | ILE | 16  | 11.550  | 17.019 | 9.697  | 1.00 | 17.47 |
| ATOM | 2348 | N   | VAL | 17  | 9.302   | 13.774 | 12.554 | 1.00 | 21.48 |
| ATOM | 2349 | CA  | VAL | 17  | 8.836   | 13.046 | 13.731 | 1.00 | 23.27 |
| ATOM | 2350 | C   | VAL | 17  | 9.225   | 13.768 | 15.021 | 1.00 | 26.50 |
| ATOM | 2351 | O   | VAL | 17  | 10.405  | 14.017 | 15.259 | 1.00 | 27.82 |
| ATOM | 2352 | CB  | VAL | 17  | 9.426   | 11.626 | 13.778 | 1.00 | 21.66 |
| ATOM | 2353 | CG1 | VAL | 17  | 8.736   | 10.805 | 14.839 | 1.00 | 19.17 |
| ATOM | 2354 | CG2 | VAL | 17  | 9.295   | 10.959 | 12.428 | 1.00 | 23.34 |
| ATOM | 2355 | H   | VAL | 17  | 10.212  | 13.598 | 12.238 | 1.00 | 0.00  |
| ATOM | 2356 | N   | GLY | 18  | 8.227   | 14.132 | 15.826 | 1.00 | 29.12 |
| ATOM | 2357 | CA  | GLY | 18  | 8.473   | 14.797 | 17.099 | 1.00 | 31.95 |
| ATOM | 2358 | C   | GLY | 18  | 8.800   | 16.288 | 17.155 | 1.00 | 34.68 |
| ATOM | 2359 | O   | GLY | 18  | 9.573   | 16.719 | 18.021 | 1.00 | 37.51 |
| ATOM | 2360 | H   | GLY | 18  | 7.319   | 13.915 | 15.553 | 1.00 | 0.00  |
| ATOM | 2361 | N   | GLY | 19  | 8.195   | 17.089 | 16.283 | 1.00 | 33.55 |
| ATOM | 2362 | CA  | GLY | 19  | 8.456   | 18.517 | 16.301 | 1.00 | 33.52 |
| ATOM | 2363 | C   | GLY | 19  | 7.175   | 19.306 | 16.126 | 1.00 | 34.87 |
| ATOM | 2364 | O   | GLY | 19  | 6.092   | 18.725 | 16.102 | 1.00 | 36.17 |
| ATOM | 2365 | H   | GLY | 19  | 7.562   | 16.732 | 15.644 | 1.00 | 0.00  |
| ATOM | 2366 | N   | GLN | 20  | 7.285   | 20.618 | 15.963 | 1.00 | 35.40 |
| ATOM | 2367 | CA  | GLN | 20  | 6.107   | 21.452 | 15.790 | 1.00 | 37.00 |
| ATOM | 2368 | C   | GLN | 20  | 6.213   | 22.229 | 14.483 | 1.00 | 36.62 |
| ATOM | 2369 | O   | GLN | 20  | 7.212   | 22.116 | 13.777 | 1.00 | 36.42 |
| ATOM | 2370 | CB  | GLN | 20  | 5.960   | 22.421 | 16.964 | 1.00 | 40.91 |
| ATOM | 2371 | CG  | GLN | 20  | 4.533   | 22.941 | 17.143 | 1.00 | 46.95 |
| ATOM | 2372 | CD  | GLN | 20  | 4.404   | 23.985 | 18.242 | 1.00 | 50.67 |
| ATOM | 2373 | OE1 | GLN | 20  | 4.648   | 23.703 | 19.418 | 1.00 | 52.08 |
| ATOM | 2374 | NE2 | GLN | 20  | 3.997   | 25.195 | 17.864 | 1.00 | 52.94 |

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|------|------|------|-----|----|--------|--------|--------|------|-------|
| ATOM | 2375 | H    | GLN | 20 | 8.174  | 21.015 | 15.889 | 1.00 | 0.00  |
| ATOM | 2376 | HE21 | GLN | 20 | 3.797  | 25.374 | 16.921 | 1.00 | 0.00  |
| ATOM | 2377 | HE22 | GLN | 20 | 3.912  | 25.857 | 18.579 | 1.00 | 0.00  |
| ATOM | 2378 | N    | GLU | 21 | 5.156  | 22.967 | 14.143 | 1.00 | 36.20 |
| ATOM | 2379 | CA   | GLU | 21 | 5.117  | 23.778 | 12.930 | 1.00 | 34.76 |
| ATOM | 2380 | C    | GLU | 21 | 6.181  | 24.844 | 13.017 | 1.00 | 33.43 |
| ATOM | 2381 | O    | GLU | 21 | 6.479  | 25.352 | 14.097 | 1.00 | 33.62 |
| ATOM | 2382 | CB   | GLU | 21 | 3.770  | 24.482 | 12.776 | 1.00 | 36.13 |
| ATOM | 2383 | CG   | GLU | 21 | 2.566  | 23.585 | 12.582 | 1.00 | 39.32 |
| ATOM | 2384 | CD   | GLU | 21 | 1.304  | 24.370 | 12.235 | 1.00 | 42.52 |
| ATOM | 2385 | OE1  | GLU | 21 | 0.198  | 23.787 | 12.329 | 1.00 | 43.84 |
| ATOM | 2386 | OE2  | GLU | 21 | 1.412  | 25.561 | 11.848 | 1.00 | 44.31 |
| ATOM | 2387 | H    | GLU | 21 | 4.352  | 22.982 | 14.689 | 1.00 | 0.00  |
| ATOM | 2388 | N    | ALA | 22 | 6.731  | 25.203 | 11.871 | 1.00 | 33.18 |
| ATOM | 2389 | CA   | ALA | 22 | 7.760  | 26.217 | 11.810 | 1.00 | 33.19 |
| ATOM | 2390 | C    | ALA | 22 | 7.104  | 27.572 | 11.605 | 1.00 | 33.14 |
| ATOM | 2391 | O    | ALA | 22 | 6.086  | 27.675 | 10.914 | 1.00 | 34.49 |
| ATOM | 2392 | CB   | ALA | 22 | 8.709  | 25.912 | 10.666 | 1.00 | 33.13 |
| ATOM | 2393 | H    | ALA | 22 | 6.433  | 24.769 | 11.053 | 1.00 | 0.00  |
| ATOM | 2394 | N    | PRO | 23 | 7.641  | 28.620 | 12.252 | 1.00 | 31.95 |
| ATOM | 2395 | CA   | PRO | 23 | 7.136  | 29.992 | 12.154 | 1.00 | 31.88 |
| ATOM | 2396 | C    | PRO | 23 | 7.145  | 30.464 | 10.702 | 1.00 | 32.61 |
| ATOM | 2397 | O    | PRO | 23 | 8.053  | 30.127 | 9.948  | 1.00 | 31.97 |
| ATOM | 2398 | CB   | PRO | 23 | 8.141  | 30.773 | 12.993 | 1.00 | 31.02 |
| ATOM | 2399 | CG   | PRO | 23 | 8.459  | 29.809 | 14.073 | 1.00 | 31.22 |
| ATOM | 2400 | CD   | PRO | 23 | 8.664  | 28.522 | 13.306 | 1.00 | 31.56 |
| ATOM | 2401 | N    | ARG | 24 | 6.169  | 31.288 | 10.332 | 1.00 | 34.96 |
| ATOM | 2402 | CA   | ARG | 24 | 6.048  | 31.790 | 8.963  | 1.00 | 38.03 |
| ATOM | 2403 | C    | ARG | 24 | 7.332  | 32.231 | 8.252  | 1.00 | 38.00 |
| ATOM | 2404 | O    | ARG | 24 | 7.347  | 32.357 | 7.026  | 1.00 | 39.29 |
| ATOM | 2405 | CB   | ARG | 24 | 4.986  | 32.896 | 8.868  | 1.00 | 41.80 |
| ATOM | 2406 | CG   | ARG | 24 | 3.587  | 32.419 | 8.426  | 1.00 | 44.91 |
| ATOM | 2407 | CD   | ARG | 24 | 2.996  | 33.291 | 7.298  | 1.00 | 46.44 |
| ATOM | 2408 | NE   | ARG | 24 | 3.260  | 32.772 | 5.948  | 1.00 | 48.09 |
| ATOM | 2409 | CZ   | ARG | 24 | 4.350  | 33.027 | 5.216  | 1.00 | 49.11 |
| ATOM | 2410 | NH1  | ARG | 24 | 5.318  | 33.805 | 5.687  | 1.00 | 48.98 |
| ATOM | 2411 | NH2  | ARG | 24 | 4.473  | 32.500 | 4.001  | 1.00 | 49.73 |
| ATOM | 2412 | H    | ARG | 24 | 5.501  | 31.539 | 11.003 | 1.00 | 0.00  |
| ATOM | 2413 | HE   | ARG | 24 | 2.544  | 32.208 | 5.583  | 1.00 | 0.00  |
| ATOM | 2414 | HH11 | ARG | 24 | 5.257  | 34.194 | 6.607  | 1.00 | 0.00  |
| ATOM | 2415 | HH12 | ARG | 24 | 6.168  | 33.962 | 5.184  | 1.00 | 0.00  |
| ATOM | 2416 | HH21 | ARG | 24 | 3.779  | 31.893 | 3.596  | 1.00 | 0.00  |
| ATOM | 2417 | HH22 | ARG | 24 | 5.275  | 32.657 | 3.420  | 1.00 | 0.00  |
| ATOM | 2418 | N    | SER | 25 | 8.394  | 32.491 | 9.000  | 1.00 | 36.70 |
| ATOM | 2419 | CA   | SER | 25 | 9.646  | 32.887 | 8.377  | 1.00 | 38.07 |
| ATOM | 2420 | C    | SER | 25 | 10.790 | 32.432 | 9.263  | 1.00 | 38.15 |
| ATOM | 2421 | O    | SER | 25 | 11.407 | 33.231 | 9.966  | 1.00 | 38.72 |
| ATOM | 2422 | CB   | SER | 25 | 9.690  | 34.400 | 8.147  | 1.00 | 39.38 |
| ATOM | 2423 | OG   | SER | 25 | 9.557  | 35.122 | 9.359  | 1.00 | 42.21 |
| ATOM | 2424 | H    | SER | 25 | 8.365  | 32.417 | 9.971  | 1.00 | 0.00  |
| ATOM | 2425 | HG   | SER | 25 | 9.067  | 34.632 | 10.019 | 1.00 | 0.00  |
| ATOM | 2426 | N    | LYS | 26 | 11.041 | 31.129 | 9.255  | 1.00 | 36.62 |
| ATOM | 2427 | CA   | LYS | 26 | 12.094 | 30.564 | 10.076 | 1.00 | 35.06 |
| ATOM | 2428 | C    | LYS | 26 | 13.086 | 29.766 | 9.245  | 1.00 | 34.73 |
| ATOM | 2429 | O    | LYS | 26 | 14.243 | 29.594 | 9.637  | 1.00 | 37.77 |
| ATOM | 2430 | CB   | LYS | 26 | 11.488 | 29.670 | 11.151 | 1.00 | 35.33 |
| ATOM | 2431 | CG   | LYS | 26 | 12.383 | 29.447 | 12.349 | 1.00 | 36.52 |
| ATOM | 2432 | CD   | LYS | 26 | 12.620 | 30.750 | 13.067 | 1.00 | 36.57 |
| ATOM | 2433 | CE   | LYS | 26 | 13.340 | 30.536 | 14.372 | 1.00 | 38.26 |
| ATOM | 2434 | NZ   | LYS | 26 | 13.409 | 31.823 | 15.116 | 1.00 | 40.27 |
| ATOM | 2435 | H    | LYS | 26 | 10.477 | 30.563 | 8.705  | 1.00 | 0.00  |
| ATOM | 2436 | H21  | LYS | 26 | 12.446 | 32.164 | 15.301 | 1.00 | 0.00  |
| ATOM | 2437 | H22  | LYS | 26 | 13.917 | 32.514 | 14.527 | 1.00 | 0.00  |

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|      |      |      |     |    |        |        |        |      |       |
|------|------|------|-----|----|--------|--------|--------|------|-------|
| ATOM | 2438 | HZ3  | LYS | 26 | 13.919 | 31.686 | 16.012 | 1.00 | 0.00  |
| ATOM | 2439 | N    | TRP | 27 | 12.642 | 29.272 | 8.099  | 1.00 | 30.07 |
| ATOM | 2440 | CA   | TRP | 27 | 13.527 | 28.493 | 7.250  | 1.00 | 26.81 |
| ATOM | 2441 | C    | TRP | 27 | 13.280 | 28.935 | 5.817  | 1.00 | 26.48 |
| ATOM | 2442 | O    | TRP | 27 | 12.693 | 28.212 | 5.022  | 1.00 | 26.57 |
| ATOM | 2443 | CB   | TRP | 27 | 13.235 | 27.001 | 7.430  | 1.00 | 24.02 |
| ATOM | 2444 | CG   | TRP | 27 | 13.038 | 26.596 | 8.866  | 1.00 | 20.50 |
| ATOM | 2445 | CD1  | TRP | 27 | 11.860 | 26.266 | 9.461  | 1.00 | 21.21 |
| ATOM | 2446 | CD2  | TRP | 27 | 14.045 | 26.475 | 9.880  | 1.00 | 19.98 |
| ATOM | 2447 | NE1  | TRP | 27 | 12.064 | 25.943 | 10.782 | 1.00 | 19.35 |
| ATOM | 2448 | CE2  | TRP | 27 | 13.395 | 26.059 | 11.066 | 1.00 | 18.90 |
| ATOM | 2449 | CE3  | TRP | 27 | 15.431 | 26.676 | 9.905  | 1.00 | 19.98 |
| ATOM | 2450 | CZ2  | TRP | 27 | 14.081 | 25.837 | 12.260 | 1.00 | 17.99 |
| ATOM | 2451 | CZ3  | TRP | 27 | 16.116 | 26.458 | 11.096 | 1.00 | 19.13 |
| ATOM | 2452 | CH2  | TRP | 27 | 15.437 | 26.039 | 12.257 | 1.00 | 19.26 |
| ATOM | 2453 | H    | TRP | 27 | 11.727 | 29.436 | 7.831  | 1.00 | 0.00  |
| ATOM | 2454 | HE1  | TRP | 27 | 11.390 | 25.696 | 11.450 | 1.00 | 0.00  |
| ATOM | 2455 | N    | PRO | 28 | 13.751 | 30.134 | 5.463  | 1.00 | 26.55 |
| ATOM | 2456 | CA   | PRO | 28 | 13.587 | 30.706 | 4.123  | 1.00 | 26.76 |
| ATOM | 2457 | C    | PRO | 28 | 14.279 | 29.954 | 3.000  | 1.00 | 26.36 |
| ATOM | 2458 | O    | PRO | 28 | 14.131 | 30.321 | 1.837  | 1.00 | 27.58 |
| ATOM | 2459 | CB   | PRO | 28 | 14.165 | 32.111 | 4.282  | 1.00 | 26.65 |
| ATOM | 2460 | CG   | PRO | 28 | 15.250 | 31.902 | 5.278  | 1.00 | 27.42 |
| ATOM | 2461 | CD   | PRO | 28 | 14.581 | 31.011 | 6.304  | 1.00 | 26.84 |
| ATOM | 2462 | N    | TRP | 29 | 15.035 | 28.916 | 3.345  | 1.00 | 25.45 |
| ATOM | 2463 | CA   | TRP | 29 | 15.750 | 28.129 | 2.341  | 1.00 | 25.13 |
| ATOM | 2464 | C    | TRP | 29 | 15.098 | 26.789 | 1.994  | 1.00 | 24.78 |
| ATOM | 2465 | O    | TRP | 29 | 15.530 | 26.120 | 1.049  | 1.00 | 25.95 |
| ATOM | 2466 | CB   | TRP | 29 | 17.194 | 27.884 | 2.784  | 1.00 | 24.26 |
| ATOM | 2467 | CG   | TRP | 29 | 17.310 | 27.230 | 4.132  | 1.00 | 22.84 |
| ATOM | 2468 | CD1  | TRP | 29 | 17.081 | 25.915 | 4.435  | 1.00 | 22.16 |
| ATOM | 2469 | CD2  | TRP | 29 | 17.669 | 27.869 | 5.360  | 1.00 | 22.18 |
| ATOM | 2470 | NE1  | TRP | 29 | 17.270 | 25.701 | 5.776  | 1.00 | 22.28 |
| ATOM | 2471 | CE2  | TRP | 29 | 17.632 | 26.882 | 6.370  | 1.00 | 22.66 |
| ATOM | 2472 | CE3  | TRP | 29 | 18.021 | 29.182 | 5.706  | 1.00 | 20.83 |
| ATOM | 2473 | CZ2  | TRP | 29 | 17.930 | 27.167 | 7.704  | 1.00 | 22.91 |
| ATOM | 2474 | CZ3  | TRP | 29 | 18.317 | 29.467 | 7.030  | 1.00 | 20.78 |
| ATOM | 2475 | CH2  | TRP | 29 | 18.269 | 28.462 | 8.014  | 1.00 | 23.06 |
| ATOM | 2476 | H    | TRP | 29 | 15.119 | 28.665 | 4.279  | 1.00 | 0.00  |
| ATOM | 2477 | HE1  | TRP | 29 | 17.126 | 24.846 | 6.245  | 1.00 | 0.00  |
| ATOM | 2478 | N    | GLN | 30 | 14.087 | 26.395 | 2.770  | 1.00 | 22.56 |
| ATOM | 2479 | CA   | GLN | 30 | 13.378 | 25.132 | 2.569  | 1.00 | 19.79 |
| ATOM | 2480 | C    | GLN | 30 | 12.780 | 25.071 | 1.168  | 1.00 | 19.70 |
| ATOM | 2481 | O    | GLN | 30 | 12.359 | 26.096 | 0.617  | 1.00 | 21.33 |
| ATOM | 2482 | CB   | GLN | 30 | 12.277 | 24.981 | 3.621  | 1.00 | 18.14 |
| ATOM | 2483 | CG   | GLN | 30 | 11.552 | 23.651 | 3.602  | 1.00 | 16.12 |
| ATOM | 2484 | CD   | GLN | 30 | 12.447 | 22.491 | 3.952  | 1.00 | 14.29 |
| ATOM | 2485 | OE1  | GLN | 30 | 12.496 | 21.497 | 3.231  | 1.00 | 15.76 |
| ATOM | 2486 | NE2  | GLN | 30 | 13.159 | 22.604 | 5.063  | 1.00 | 11.06 |
| ATOM | 2487 | H    | GLN | 30 | 13.745 | 26.996 | 3.457  | 1.00 | 0.00  |
| ATOM | 2488 | HE21 | GLN | 30 | 13.100 | 23.413 | 5.605  | 1.00 | 0.00  |
| ATOM | 2489 | HE22 | GLN | 30 | 13.720 | 21.832 | 5.270  | 1.00 | 0.00  |
| ATOM | 2490 | N    | VAL | 31 | 12.759 | 23.876 | 0.592  | 1.00 | 18.32 |
| ATOM | 2491 | CA   | VAL | 31 | 12.228 | 23.678 | -0.750 | 1.00 | 17.12 |
| ATOM | 2492 | C    | VAL | 31 | 11.439 | 22.375 | -0.845 | 1.00 | 16.16 |
| ATOM | 2493 | O    | VAL | 31 | 11.690 | 21.430 | -0.092 | 1.00 | 16.44 |
| ATOM | 2494 | CB   | VAL | 31 | 13.375 | 23.690 | -1.799 | 1.00 | 16.99 |
| ATOM | 2495 | CG1  | VAL | 31 | 12.932 | 23.065 | -3.107 | 1.00 | 17.45 |
| ATOM | 2496 | CG2  | VAL | 31 | 13.832 | 25.119 | -2.052 | 1.00 | 18.64 |
| ATOM | 2497 | H    | VAL | 31 | 13.122 | 23.086 | 1.052  | 1.00 | 0.00  |
| ATOM | 2498 | N    | SER | 32 | 10.445 | 22.367 | -1.728 | 1.00 | 14.09 |
| ATOM | 2499 | CA   | SER | 32 | 9.609  | 21.205 | -1.971 | 1.00 | 13.42 |
| ATOM | 2500 | C    | SER | 32 | 9.792  | 20.816 | -3.428 | 1.00 | 13.80 |

|      |      |      |     |     |        |        |         |      |       |
|------|------|------|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2501 | O    | SER | 32  | 9.605  | 21.649 | -4.313  | 1.00 | 15.20 |
| ATOM | 2502 | CB   | SER | 32  | 8.141  | 21.544 | -1.716  | 1.00 | 13.19 |
| ATOM | 2503 | OG   | SER | 32  | 7.288  | 20.484 | -2.125  | 1.00 | 12.32 |
| ATOM | 2504 | H    | SER | 32  | 10.255 | 23.191 | -2.219  | 1.00 | 0.00  |
| ATOM | 2505 | HG   | SER | 32  | 6.372  | 20.719 | -1.909  | 1.00 | 0.00  |
| ATOM | 2506 | N    | LEU | 33  | 10.233 | 19.585 | -3.667  | 1.00 | 13.20 |
| ATOM | 2507 | CA   | LEU | 33  | 10.428 | 19.085 | -5.020  | 1.00 | 13.21 |
| ATOM | 2508 | C    | LEU | 33  | 9.149  | 18.369 | -5.394  | 1.00 | 15.47 |
| ATOM | 2509 | O    | LEU | 33  | 8.661  | 17.535 | -4.622  | 1.00 | 16.81 |
| ATOM | 2510 | CB   | LEU | 33  | 11.604 | 18.111 | -5.085  | 1.00 | 12.12 |
| ATOM | 2511 | CG   | LEU | 33  | 13.004 | 18.616 | -4.739  | 1.00 | 11.95 |
| ATOM | 2512 | CD1  | LEU | 33  | 14.048 | 17.626 | -5.256  | 1.00 | 10.82 |
| ATOM | 2513 | CD2  | LEU | 33  | 13.227 | 19.984 | -5.353  | 1.00 | 11.27 |
| ATOM | 2514 | H    | LEU | 33  | 10.429 | 19.005 | -2.915  | 1.00 | 0.00  |
| ATOM | 2515 | N    | ARG | 34  | 8.618  | 18.671 | -6.575  | 1.00 | 16.91 |
| ATOM | 2516 | CA   | ARG | 34  | 7.370  | 18.069 | -7.031  | 1.00 | 19.06 |
| ATOM | 2517 | C    | ARG | 34  | 7.516  | 17.201 | -8.280  | 1.00 | 21.65 |
| ATOM | 2518 | O    | ARG | 34  | 8.478  | 17.342 | -9.036  | 1.00 | 23.43 |
| ATOM | 2519 | CB   | ARG | 34  | 6.354  | 19.167 | -7.340  | 1.00 | 17.58 |
| ATOM | 2520 | CG   | ARG | 34  | 6.261  | 20.267 | -6.318  | 1.00 | 16.22 |
| ATOM | 2521 | CD   | ARG | 34  | 5.594  | 19.814 | -5.036  | 1.00 | 16.92 |
| ATOM | 2522 | NE   | ARG | 34  | 5.360  | 20.971 | -4.173  | 1.00 | 18.23 |
| ATOM | 2523 | CZ   | ARG | 34  | 4.220  | 21.660 | -4.115  | 1.00 | 17.31 |
| ATOM | 2524 | NH1  | ARG | 34  | 3.171  | 21.309 | -4.854  | 1.00 | 16.04 |
| ATOM | 2525 | NH2  | ARG | 34  | 4.132  | 22.717 | -3.315  | 1.00 | 18.61 |
| ATOM | 2526 | H    | ARG | 34  | 9.083  | 19.302 | -7.162  | 1.00 | 0.00  |
| ATOM | 2527 | HE   | ARG | 34  | 6.127  | 21.197 | -3.616  | 1.00 | 0.00  |
| ATOM | 2528 | HH11 | ARG | 34  | 3.136  | 20.499 | -5.443  | 1.00 | 0.00  |
| ATOM | 2529 | HH12 | ARG | 34  | 2.344  | 21.904 | -4.839  | 1.00 | 0.00  |
| ATOM | 2530 | HH21 | ARG | 34  | 4.824  | 23.118 | -2.714  | 1.00 | 0.00  |
| ATOM | 2531 | HH22 | ARG | 34  | 3.269  | 23.270 | -3.296  | 1.00 | 0.00  |
| ATOM | 2532 | N    | VAL | 35  | 6.544  | 16.311 | -8.485  | 1.00 | 23.39 |
| ATOM | 2533 | CA   | VAL | 35  | 6.487  | 15.439 | -9.656  | 1.00 | 25.24 |
| ATOM | 2534 | C    | VAL | 35  | 5.079  | 15.486 | -10.208 | 1.00 | 29.75 |
| ATOM | 2535 | O    | VAL | 35  | 4.102  | 15.568 | -9.451  | 1.00 | 29.19 |
| ATOM | 2536 | CB   | VAL | 35  | 6.809  | 13.970 | -9.354  | 1.00 | 22.92 |
| ATOM | 2537 | CG1  | VAL | 35  | 8.289  | 13.756 | -9.358  | 1.00 | 24.74 |
| ATOM | 2538 | CG2  | VAL | 35  | 6.200  | 13.546 | -8.039  | 1.00 | 22.83 |
| ATOM | 2539 | H    | VAL | 35  | 5.841  | 16.248 | -7.804  | 1.00 | 0.00  |
| ATOM | 2540 | N    | HIS | 36  | 4.992  | 15.403 | -11.532 | 1.00 | 34.90 |
| ATOM | 2541 | CA   | HIS | 36  | 3.728  | 15.445 | -12.251 | 1.00 | 39.85 |
| ATOM | 2542 | C    | HIS | 36  | 2.504  | 14.880 | -11.533 | 1.00 | 40.09 |
| ATOM | 2543 | O    | HIS | 36  | 1.666  | 15.649 | -11.079 | 1.00 | 42.12 |
| ATOM | 2544 | CB   | HIS | 36  | 3.873  | 14.865 | -13.670 | 1.00 | 48.03 |
| ATOM | 2545 | CG   | HIS | 36  | 4.247  | 13.407 | -13.722 | 1.00 | 56.59 |
| ATOM | 2546 | ND1  | HIS | 36  | 5.437  | 12.911 | -13.226 | 1.00 | 59.53 |
| ATOM | 2547 | CD2  | HIS | 36  | 3.598  | 12.344 | -14.263 | 1.00 | 59.06 |
| ATOM | 2548 | CE1  | HIS | 36  | 5.505  | 11.611 | -13.459 | 1.00 | 60.32 |
| ATOM | 2549 | NE2  | HIS | 36  | 4.403  | 11.243 | -14.088 | 1.00 | 60.67 |
| ATOM | 2550 | H    | HIS | 36  | 5.840  | 15.437 | -12.013 | 1.00 | 0.00  |
| ATOM | 2551 | HD1  | HIS | 36  | 6.202  | 13.362 | -12.790 | 1.00 | 0.00  |
| ATOM | 2552 | HE2  | HIS | 36  | 4.194  | 10.338 | -14.407 | 1.00 | 0.00  |
| ATOM | 2553 | N    | GLY | 37  | 2.403  | 13.559 | -11.408 | 1.00 | 38.78 |
| ATOM | 2554 | CA   | GLY | 37  | 1.248  | 12.964 | -10.743 | 1.00 | 38.47 |
| ATOM | 2555 | C    | GLY | 37  | -0.096 | 13.228 | -11.422 | 1.00 | 36.88 |
| ATOM | 2556 | O    | GLY | 37  | -0.129 | 13.644 | -12.580 | 1.00 | 37.63 |
| ATOM | 2557 | H    | GLY | 37  | 3.105  | 12.971 | -11.713 | 1.00 | 0.00  |
| ATOM | 2558 | N    | PRO | 37A | -1.226 | 12.954 | -10.740 | 1.00 | 35.09 |
| ATOM | 2559 | CA   | PRO | 37A | -2.480 | 13.700 | -10.906 | 1.00 | 33.69 |
| ATOM | 2560 | C    | PRO | 37A | -2.324 | 15.161 | -10.497 | 1.00 | 32.82 |
| ATOM | 2561 | O    | PRO | 37A | -3.130 | 16.012 | -10.865 | 1.00 | 32.88 |
| ATOM | 2562 | CB   | PRO | 37A | -3.433 | 12.973 | -9.962  | 1.00 | 33.08 |
| ATOM | 2563 | CG   | PRO | 37A | -2.909 | 11.584 | -9.955  | 1.00 | 33.35 |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2564 | CD  | PRO | 37A | -1.429 | 11.804 | -9.845  | 1.00 | 34.14 |
| ATOM | 2565 | N   | TYR | 37B | -1.309 | 15.429 | -9.686  | 1.00 | 31.45 |
| ATOM | 2566 | CA  | TYR | 37B | -1.022 | 16.776 | -9.225  | 1.00 | 30.81 |
| ATOM | 2567 | C   | TYR | 37B | 0.453  | 16.838 | -8.859  | 1.00 | 31.27 |
| ATOM | 2568 | O   | TYR | 37B | 1.084  | 15.809 | -8.581  | 1.00 | 32.71 |
| ATOM | 2569 | CB  | TYR | 37B | -1.881 | 17.142 | -8.011  | 1.00 | 28.47 |
| ATOM | 2570 | CG  | TYR | 37B | -1.623 | 16.309 | -6.772  | 1.00 | 28.52 |
| ATOM | 2571 | CD1 | TYR | 37B | -0.927 | 16.835 | -5.685  | 1.00 | 28.66 |
| ATOM | 2572 | CD2 | TYR | 37B | -2.107 | 15.008 | -6.670  | 1.00 | 29.80 |
| ATOM | 2573 | CE1 | TYR | 37B | -0.726 | 16.082 | -4.527  | 1.00 | 28.84 |
| ATOM | 2574 | CE2 | TYR | 37B | -1.912 | 14.249 | -5.513  | 1.00 | 29.05 |
| ATOM | 2575 | CZ  | TYR | 37B | -1.225 | 14.793 | -4.450  | 1.00 | 28.75 |
| ATOM | 2576 | OH  | TYR | 37B | -1.064 | 14.054 | -3.299  | 1.00 | 30.25 |
| ATOM | 2577 | H   | TYR | 37B | -0.674 | 14.741 | -9.401  | 1.00 | 0.00  |
| ATOM | 2578 | HH  | TYR | 37B | -0.442 | 14.569 | -2.765  | 1.00 | 0.00  |
| ATOM | 2579 | N   | TRP | 38  | 1.002  | 18.045 | -8.875  | 1.00 | 29.57 |
| ATOM | 2580 | CA  | TRP | 38  | 2.395  | 18.258 | -8.535  | 1.00 | 27.83 |
| ATOM | 2581 | C   | TRP | 38  | 2.636  | 17.823 | -7.102  | 1.00 | 27.67 |
| ATOM | 2582 | O   | TRP | 38  | 2.667  | 18.633 | -6.172  | 1.00 | 27.98 |
| ATOM | 2583 | CB  | TRP | 38  | 2.738  | 19.719 | -8.756  | 1.00 | 27.58 |
| ATOM | 2584 | CG  | TRP | 38  | 2.673  | 20.045 | -10.193 | 1.00 | 27.51 |
| ATOM | 2585 | CD1 | TRP | 38  | 1.665  | 20.691 | -10.844 | 1.00 | 26.98 |
| ATOM | 2586 | CD2 | TRP | 38  | 3.627  | 19.665 | -11.194 | 1.00 | 27.86 |
| ATOM | 2587 | NE1 | TRP | 38  | 1.927  | 20.728 | -12.192 | 1.00 | 27.54 |
| ATOM | 2588 | CE2 | TRP | 38  | 3.128  | 20.109 | -12.434 | 1.00 | 27.71 |
| ATOM | 2589 | CE3 | TRP | 38  | 4.858  | 18.990 | -11.161 | 1.00 | 27.01 |
| ATOM | 2590 | CZ2 | TRP | 38  | 3.817  | 19.899 | -13.638 | 1.00 | 27.95 |
| ATOM | 2591 | CZ3 | TRP | 38  | 5.539  | 18.784 | -12.357 | 1.00 | 27.43 |
| ATOM | 2592 | CH2 | TRP | 38  | 5.016  | 19.238 | -13.579 | 1.00 | 27.02 |
| ATOM | 2593 | H   | TRP | 38  | 0.448  | 18.808 | -9.123  | 1.00 | 0.00  |
| ATOM | 2594 | HE1 | TRP | 38  | 1.328  | 21.111 | -12.868 | 1.00 | 0.00  |
| ATOM | 2595 | N   | MET | 39  | 2.836  | 16.525 | -6.955  | 1.00 | 27.45 |
| ATOM | 2596 | CA  | MET | 39  | 3.039  | 15.888 | -5.674  | 1.00 | 28.88 |
| ATOM | 2597 | C   | MET | 39  | 4.417  | 16.177 | -5.078  | 1.00 | 28.83 |
| ATOM | 2598 | O   | MET | 39  | 5.414  | 16.207 | -5.802  | 1.00 | 30.54 |
| ATOM | 2599 | CB  | MET | 39  | 2.873  | 14.391 | -5.886  | 1.00 | 31.85 |
| ATOM | 2600 | CG  | MET | 39  | 2.399  | 13.616 | -4.692  | 1.00 | 34.61 |
| ATOM | 2601 | SD  | MET | 39  | 2.224  | 11.903 | -5.183  | 1.00 | 37.58 |
| ATOM | 2602 | CE  | MET | 39  | 1.325  | 12.088 | -6.775  | 1.00 | 35.07 |
| ATOM | 2603 | H   | MET | 39  | 2.895  | 15.993 | -7.783  | 1.00 | 0.00  |
| ATOM | 2604 | N   | HIS | 40  | 4.465  | 16.430 | -3.770  | 1.00 | 25.91 |
| ATOM | 2605 | CA  | HIS | 40  | 5.732  | 16.680 | -3.077  | 1.00 | 23.53 |
| ATOM | 2606 | C   | HIS | 40  | 6.411  | 15.335 | -2.854  | 1.00 | 22.49 |
| ATOM | 2607 | O   | HIS | 40  | 5.818  | 14.460 | -2.223  | 1.00 | 24.35 |
| ATOM | 2608 | CB  | HIS | 40  | 5.482  | 17.342 | -1.709  | 1.00 | 21.80 |
| ATOM | 2609 | CG  | HIS | 40  | 6.626  | 17.214 | -0.743  | 1.00 | 19.85 |
| ATOM | 2610 | ND1 | HIS | 40  | 7.636  | 18.144 | -0.655  | 1.00 | 19.82 |
| ATOM | 2611 | CD2 | HIS | 40  | 6.925  | 16.252 | 0.165   | 1.00 | 19.92 |
| ATOM | 2612 | CE1 | HIS | 40  | 8.511  | 17.765 | 0.259   | 1.00 | 19.50 |
| ATOM | 2613 | NE2 | HIS | 40  | 8.104  | 16.618 | 0.771   | 1.00 | 19.97 |
| ATOM | 2614 | H   | HIS | 40  | 3.627  | 16.493 | -3.265  | 1.00 | 0.00  |
| ATOM | 2615 | HD1 | HIS | 40  | 7.692  | 18.959 | -1.198  | 1.00 | 0.00  |
| ATOM | 2616 | HE2 | HIS | 40  | 8.620  | 16.094 | 1.430   | 1.00 | 0.00  |
| ATOM | 2617 | N   | PHE | 41  | 7.641  | 15.163 | -3.335  | 1.00 | 19.65 |
| ATOM | 2618 | CA  | PHE | 41  | 8.345  | 13.896 | -3.122  | 1.00 | 17.53 |
| ATOM | 2619 | C   | PHE | 41  | 9.585  | 14.014 | -2.227  | 1.00 | 16.64 |
| ATOM | 2620 | O   | PHE | 41  | 10.013 | 13.045 | -1.599  | 1.00 | 15.87 |
| ATOM | 2621 | CB  | PHE | 41  | 8.672  | 13.190 | -4.461  | 1.00 | 16.21 |
| ATOM | 2622 | CG  | PHE | 41  | 9.729  | 13.875 | -5.302  | 1.00 | 15.02 |
| ATOM | 2623 | CD1 | PHE | 41  | 11.068 | 13.529 | -5.179  | 1.00 | 13.68 |
| ATOM | 2624 | CD2 | PHE | 41  | 9.382  | 14.833 | -6.243  | 1.00 | 15.50 |
| ATOM | 2625 | CE1 | PHE | 41  | 12.040 | 14.125 | -5.977  | 1.00 | 13.28 |
| ATOM | 2626 | CE2 | PHE | 41  | 10.357 | 15.432 | -7.047  | 1.00 | 15.21 |

|      |      |     |     |    |        |        |        |      |       |
|------|------|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 2627 | CZ  | PHE | 41 | 11.686 | 15.075 | -6.910 | 1.00 | 13.41 |
| ATOM | 2628 | H   | PHE | 41 | 8.037  | 15.900 | -3.847 | 1.00 | 0.00  |
| ATOM | 2629 | N   | CYS | 42 | 10.108 | 15.226 | -2.106 | 1.00 | 16.41 |
| ATOM | 2630 | CA  | CYS | 42 | 11.295 | 15.468 | -1.305 | 1.00 | 15.51 |
| ATOM | 2631 | C   | CYS | 42 | 11.450 | 16.939 | -0.995 | 1.00 | 16.13 |
| ATOM | 2632 | O   | CYS | 42 | 10.766 | 17.782 | -1.577 | 1.00 | 17.43 |
| ATOM | 2633 | CB  | CYS | 42 | 12.527 | 15.022 | -2.072 | 1.00 | 13.97 |
| ATOM | 2634 | SG  | CYS | 42 | 12.861 | 13.250 | -1.978 | 1.00 | 13.42 |
| ATOM | 2635 | H   | CYS | 42 | 9.721  | 15.976 | -2.597 | 1.00 | 0.00  |
| ATOM | 2636 | N   | GLY | 43 | 12.358 | 17.239 | -0.080 | 1.00 | 15.27 |
| ATOM | 2637 | CA  | GLY | 43 | 12.609 | 18.612 | 0.290  | 1.00 | 15.57 |
| ATOM | 2638 | C   | GLY | 43 | 13.929 | 18.982 | -0.330 | 1.00 | 17.30 |
| ATOM | 2639 | O   | GLY | 43 | 14.477 | 18.211 | -1.122 | 1.00 | 19.14 |
| ATOM | 2640 | H   | GLY | 43 | 12.929 | 16.526 | 0.285  | 1.00 | 0.00  |
| ATOM | 2641 | N   | GLY | 44 | 14.447 | 20.146 | 0.040  | 1.00 | 17.05 |
| ATOM | 2642 | CA  | GLY | 44 | 15.721 | 20.605 | -0.485 | 1.00 | 17.02 |
| ATOM | 2643 | C   | GLY | 44 | 16.006 | 21.969 | 0.100  | 1.00 | 17.99 |
| ATOM | 2644 | O   | GLY | 44 | 15.235 | 22.446 | 0.935  | 1.00 | 19.89 |
| ATOM | 2645 | H   | GLY | 44 | 13.969 | 20.713 | 0.677  | 1.00 | 0.00  |
| ATOM | 2646 | N   | SER | 45 | 17.105 | 22.594 | -0.297 | 1.00 | 17.11 |
| ATOM | 2647 | CA  | SER | 45 | 17.423 | 23.918 | 0.213  | 1.00 | 17.01 |
| ATOM | 2648 | C   | SER | 45 | 18.030 | 24.784 | -0.866 | 1.00 | 17.61 |
| ATOM | 2649 | O   | SER | 45 | 18.636 | 24.278 | -1.814 | 1.00 | 19.51 |
| ATOM | 2650 | CB  | SER | 45 | 18.381 | 23.823 | 1.391  | 1.00 | 17.98 |
| ATOM | 2651 | OG  | SER | 45 | 19.564 | 23.162 | 1.003  | 1.00 | 21.12 |
| ATOM | 2652 | H   | SER | 45 | 17.735 | 22.124 | -0.887 | 1.00 | 0.00  |
| ATOM | 2653 | HG  | SER | 45 | 20.281 | 23.346 | 1.622  | 1.00 | 0.00  |
| ATOM | 2654 | N   | LEU | 46 | 17.826 | 26.087 | -0.739 | 1.00 | 17.02 |
| ATOM | 2655 | CA  | LEU | 46 | 18.359 | 27.052 | -1.689 | 1.00 | 17.24 |
| ATOM | 2656 | C   | LEU | 46 | 19.774 | 27.389 | -1.223 | 1.00 | 19.59 |
| ATOM | 2657 | O   | LEU | 46 | 19.949 | 28.114 | -0.245 | 1.00 | 21.65 |
| ATOM | 2658 | CB  | LEU | 46 | 17.490 | 28.302 | -1.658 | 1.00 | 14.31 |
| ATOM | 2659 | CG  | LEU | 46 | 17.444 | 29.197 | -2.882 | 1.00 | 10.66 |
| ATOM | 2660 | CD1 | LEU | 46 | 16.885 | 28.416 | -4.041 | 1.00 | 8.44  |
| ATOM | 2661 | CD2 | LEU | 46 | 16.562 | 30.389 | -2.572 | 1.00 | 9.92  |
| ATOM | 2662 | H   | LEU | 46 | 17.269 | 26.385 | 0.007  | 1.00 | 0.00  |
| ATOM | 2663 | N   | ILE | 47 | 20.789 | 26.839 | -1.882 | 1.00 | 20.63 |
| ATOM | 2664 | CA  | ILE | 47 | 22.166 | 27.108 | -1.475 | 1.00 | 21.59 |
| ATOM | 2665 | C   | ILE | 47 | 22.809 | 28.261 | -2.243 | 1.00 | 26.00 |
| ATOM | 2666 | O   | ILE | 47 | 23.941 | 28.657 | -1.956 | 1.00 | 28.12 |
| ATOM | 2667 | CB  | ILE | 47 | 23.040 | 25.860 | -1.609 | 1.00 | 18.83 |
| ATOM | 2668 | CG1 | ILE | 47 | 23.199 | 25.474 | -3.082 | 1.00 | 17.78 |
| ATOM | 2669 | CG2 | ILE | 47 | 22.426 | 24.729 | -0.812 | 1.00 | 19.00 |
| ATOM | 2670 | H   | ILE | 47 | 20.574 | 26.259 | -2.650 | 1.00 | 0.00  |
| ATOM | 2671 | CD  | ILE | 47 | 24.117 | 24.279 | -3.329 | 1.00 | 15.97 |
| ATOM | 2672 | N   | HIS | 48 | 22.063 | 28.812 | -3.197 | 1.00 | 28.50 |
| ATOM | 2673 | CA  | HIS | 48 | 22.507 | 29.919 | -4.048 | 1.00 | 29.64 |
| ATOM | 2674 | C   | HIS | 48 | 21.244 | 30.318 | -4.802 | 1.00 | 30.24 |
| ATOM | 2675 | O   | HIS | 48 | 20.396 | 29.470 | -5.071 | 1.00 | 30.81 |
| ATOM | 2676 | CB  | HIS | 48 | 23.581 | 29.422 | -5.026 | 1.00 | 31.70 |
| ATOM | 2677 | CG  | HIS | 48 | 24.036 | 30.448 | -6.018 | 1.00 | 33.16 |
| ATOM | 2678 | ND1 | HIS | 48 | 25.240 | 31.110 | -5.904 | 1.00 | 34.00 |
| ATOM | 2679 | CD2 | HIS | 48 | 23.466 | 30.901 | -7.161 | 1.00 | 32.66 |
| ATOM | 2680 | CE1 | HIS | 48 | 25.392 | 31.925 | -6.932 | 1.00 | 35.23 |
| ATOM | 2681 | NE2 | HIS | 48 | 24.330 | 31.816 | -7.710 | 1.00 | 33.30 |
| ATOM | 2682 | H   | HIS | 48 | 21.159 | 28.462 | -3.362 | 1.00 | 0.00  |
| ATOM | 2683 | HD1 | HIS | 48 | 25.904 | 30.997 | -5.169 | 1.00 | 0.00  |
| ATOM | 2684 | HE2 | HIS | 48 | 24.209 | 32.306 | -8.554 | 1.00 | 0.00  |
| ATOM | 2685 | N   | PRO | 49 | 21.104 | 31.598 | -5.173 | 1.00 | 30.34 |
| ATOM | 2686 | CA  | PRO | 49 | 19.912 | 32.056 | -5.897 | 1.00 | 30.07 |
| ATOM | 2687 | C   | PRO | 49 | 19.492 | 31.326 | -7.187 | 1.00 | 29.56 |
| ATOM | 2688 | O   | PRO | 49 | 18.592 | 31.792 | -7.875 | 1.00 | 31.26 |
| ATOM | 2689 | CB  | PRO | 49 | 20.233 | 33.525 | -6.166 | 1.00 | 29.78 |

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|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 2690 | CG   | PRO | 49 | 21.000 | 33.915 | -4.954  | 1.00 | 29.91 |
| ATOM | 2691 | CD   | PRO | 49 | 21.950 | 32.747 | -4.800  | 1.00 | 31.01 |
| ATOM | 2692 | N    | GLN | 50 | 20.099 | 30.188 | -7.511  | 1.00 | 27.66 |
| ATOM | 2693 | CA   | GLN | 50 | 19.724 | 29.481 | -8.733  | 1.00 | 26.78 |
| ATOM | 2694 | C    | GLN | 50 | 20.006 | 27.979 | -8.707  | 1.00 | 25.56 |
| ATOM | 2695 | O    | GLN | 50 | 19.869 | 27.288 | -9.719  | 1.00 | 26.68 |
| ATOM | 2696 | CB   | GLN | 50 | 20.415 | 30.118 | -9.934  | 1.00 | 28.29 |
| ATOM | 2697 | CG   | GLN | 50 | 19.857 | 29.663 | -11.266 | 1.00 | 31.10 |
| ATOM | 2698 | CD   | GLN | 50 | 20.549 | 30.314 | -12.434 | 1.00 | 32.60 |
| ATOM | 2699 | OE1  | GLN | 50 | 21.479 | 31.106 | -12.258 | 1.00 | 34.73 |
| ATOM | 2700 | NE2  | GLN | 50 | 20.107 | 29.981 | -13.640 | 1.00 | 32.63 |
| ATOM | 2701 | H    | GLN | 50 | 20.762 | 29.768 | -6.949  | 1.00 | 0.00  |
| ATOM | 2702 | HE21 | GLN | 50 | 19.396 | 29.305 | -13.699 | 1.00 | 0.00  |
| ATOM | 2703 | HE22 | GLN | 50 | 20.518 | 30.403 | -14.419 | 1.00 | 0.00  |
| ATOM | 2704 | N    | TRP | 51 | 20.360 | 27.467 | -7.540  | 1.00 | 22.55 |
| ATOM | 2705 | CA   | TRP | 51 | 20.645 | 26.055 | -7.403  | 1.00 | 20.61 |
| ATOM | 2706 | C    | TRP | 51 | 19.932 | 25.533 | -6.187  | 1.00 | 20.60 |
| ATOM | 2707 | O    | TRP | 51 | 19.655 | 26.275 | -5.249  | 1.00 | 21.95 |
| ATOM | 2708 | CB   | TRP | 51 | 22.135 | 25.831 | -7.225  | 1.00 | 20.58 |
| ATOM | 2709 | CG   | TRP | 51 | 22.913 | 26.065 | -8.442  | 1.00 | 21.12 |
| ATOM | 2710 | CD1  | TRP | 51 | 23.459 | 27.243 | -8.853  | 1.00 | 20.74 |
| ATOM | 2711 | CD2  | TRP | 51 | 23.261 | 25.091 | -9.426  | 1.00 | 21.74 |
| ATOM | 2712 | NE1  | TRP | 51 | 24.132 | 27.062 | -10.037 | 1.00 | 22.47 |
| ATOM | 2713 | CE2  | TRP | 51 | 24.026 | 25.748 | -10.411 | 1.00 | 21.72 |
| ATOM | 2714 | CE3  | TRP | 51 | 23.000 | 23.723 | -9.569  | 1.00 | 22.40 |
| ATOM | 2715 | CZ2  | TRP | 51 | 24.538 | 25.087 | -11.530 | 1.00 | 22.08 |
| ATOM | 2716 | CZ3  | TRP | 51 | 23.511 | 23.061 | -10.684 | 1.00 | 23.51 |
| ATOM | 2717 | CH2  | TRP | 51 | 24.271 | 23.747 | -11.650 | 1.00 | 22.85 |
| ATOM | 2718 | H    | TRP | 51 | 20.359 | 28.006 | -6.724  | 1.00 | 0.00  |
| ATOM | 2719 | HE1  | TRP | 51 | 24.588 | 27.744 | -10.577 | 1.00 | 0.00  |
| ATOM | 2720 | N    | VAL | 52 | 19.642 | 24.246 | -6.194  | 1.00 | 20.29 |
| ATOM | 2721 | CA   | VAL | 52 | 18.977 | 23.631 | -5.070  | 1.00 | 20.05 |
| ATOM | 2722 | C    | VAL | 52 | 19.770 | 22.384 | -4.722  | 1.00 | 19.26 |
| ATOM | 2723 | O    | VAL | 52 | 20.294 | 21.699 | -5.608  | 1.00 | 18.68 |
| ATOM | 2724 | CB   | VAL | 52 | 17.521 | 23.267 | -5.415  | 1.00 | 21.89 |
| ATOM | 2725 | CG1  | VAL | 52 | 16.800 | 22.733 | -4.185  | 1.00 | 23.63 |
| ATOM | 2726 | CG2  | VAL | 52 | 16.792 | 24.488 | -5.957  | 1.00 | 22.79 |
| ATOM | 2727 | H    | VAL | 52 | 19.849 | 23.708 | -6.986  | 1.00 | 0.00  |
| ATOM | 2728 | N    | LEU | 53 | 19.927 | 22.151 | -3.426  | 1.00 | 18.21 |
| ATOM | 2729 | CA   | LEU | 53 | 20.655 | 20.995 | -2.931  | 1.00 | 17.23 |
| ATOM | 2730 | C    | LEU | 53 | 19.628 | 19.984 | -2.434  | 1.00 | 17.42 |
| ATOM | 2731 | O    | LEU | 53 | 18.676 | 20.343 | -1.735  | 1.00 | 17.68 |
| ATOM | 2732 | CB   | LEU | 53 | 21.604 | 21.423 | -1.807  | 1.00 | 15.02 |
| ATOM | 2733 | CG   | LEU | 53 | 22.556 | 20.410 | -1.177  | 1.00 | 12.62 |
| ATOM | 2734 | CD1  | LEU | 53 | 23.370 | 19.700 | -2.234  | 1.00 | 12.84 |
| ATOM | 2735 | CD2  | LEU | 53 | 23.459 | 21.137 | -0.210  | 1.00 | 12.00 |
| ATOM | 2736 | H    | LEU | 53 | 19.536 | 22.787 | -2.792  | 1.00 | 0.00  |
| ATOM | 2737 | N    | THR | 54 | 19.802 | 18.732 | -2.827  | 1.00 | 17.53 |
| ATOM | 2738 | CA   | THR | 54 | 18.878 | 17.684 | -2.436  | 1.00 | 19.37 |
| ATOM | 2739 | C    | THR | 54 | 19.627 | 16.368 | -2.412  | 1.00 | 20.64 |
| ATOM | 2740 | O    | THR | 54 | 20.732 | 16.270 | -2.949  | 1.00 | 22.18 |
| ATOM | 2741 | CB   | THR | 54 | 17.708 | 17.573 | -3.444  | 1.00 | 19.81 |
| ATOM | 2742 | OG1  | THR | 54 | 16.767 | 16.593 | -2.990  | 1.00 | 20.34 |
| ATOM | 2743 | CG2  | THR | 54 | 18.222 | 17.172 | -4.823  | 1.00 | 18.84 |
| ATOM | 2744 | H    | THR | 54 | 20.562 | 18.501 | -3.407  | 1.00 | 0.00  |
| ATOM | 2745 | HG1  | THR | 54 | 17.052 | 15.713 | -3.244  | 1.00 | 0.00  |
| ATOM | 2746 | N    | ALA | 55 | 19.032 | 15.369 | -1.766  | 1.00 | 20.18 |
| ATOM | 2747 | CA   | ALA | 55 | 19.622 | 14.040 | -1.678  | 1.00 | 19.11 |
| ATOM | 2748 | C    | ALA | 55 | 19.480 | 13.435 | -3.067  | 1.00 | 19.11 |
| ATOM | 2749 | O    | ALA | 55 | 18.418 | 13.518 | -3.684  | 1.00 | 19.41 |
| ATOM | 2750 | CB   | ALA | 55 | 18.881 | 13.191 | -0.645  | 1.00 | 17.89 |
| ATOM | 2751 | H    | ALA | 55 | 18.154 | 15.567 | -1.391  | 1.00 | 0.00  |
| ATOM | 2752 | N    | ALA | 56 | 20.555 | 12.841 | -3.563  | 1.00 | 18.83 |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2753 | CA  | ALA | 56  | 20.552 | 12.249 | -4.886  | 1.00 | 17.36 |
| ATOM | 2754 | C   | ALA | 56  | 19.450 | 11.221 | -5.051  | 1.00 | 17.46 |
| ATOM | 2755 | O   | ALA | 56  | 18.778 | 11.198 | -6.076  | 1.00 | 18.33 |
| ATOM | 2756 | CB  | ALA | 56  | 21.892 | 11.624 | -5.179  | 1.00 | 16.53 |
| ATOM | 2757 | H   | ALA | 56  | 21.351 | 12.744 | -2.995  | 1.00 | 0.00  |
| ATOM | 2758 | N   | HIS | 57  | 19.200 | 10.424 | -4.019  | 1.00 | 17.19 |
| ATOM | 2759 | CA  | HIS | 57  | 18.180 | 9.388  | -4.135  | 1.00 | 17.54 |
| ATOM | 2760 | C   | HIS | 57  | 16.794 | 9.884  | -4.509  | 1.00 | 17.73 |
| ATOM | 2761 | O   | HIS | 57  | 15.974 | 9.104  | -5.003  | 1.00 | 19.07 |
| ATOM | 2762 | CB  | HIS | 57  | 18.140 | 8.458  | -2.912  | 1.00 | 15.19 |
| ATOM | 2763 | CG  | HIS | 57  | 17.451 | 9.028  | -1.716  | 1.00 | 13.02 |
| ATOM | 2764 | ND1 | HIS | 57  | 18.109 | 9.781  | -0.770  | 1.00 | 14.48 |
| ATOM | 2765 | CD2 | HIS | 57  | 16.182 | 8.885  | -1.266  | 1.00 | 12.46 |
| ATOM | 2766 | CE1 | HIS | 57  | 17.280 | 10.071 | 0.217   | 1.00 | 14.99 |
| ATOM | 2767 | NE2 | HIS | 57  | 16.104 | 9.540  | -0.060  | 1.00 | 13.56 |
| ATOM | 2768 | H   | HIS | 57  | 19.735 | 10.539 | -3.222  | 1.00 | 0.00  |
| ATOM | 2769 | HD1 | HIS | 57  | 19.029 | 10.101 | -0.797  | 1.00 | 0.00  |
| ATOM | 2770 | HE2 | HIS | 57  | 15.364 | 9.660  | 0.589   | 1.00 | 0.00  |
| ATOM | 2771 | N   | CYS | 58  | 16.557 | 11.183 | -4.325  | 1.00 | 15.90 |
| ATOM | 2772 | CA  | CYS | 58  | 15.270 | 11.781 | -4.664  | 1.00 | 13.65 |
| ATOM | 2773 | C   | CYS | 58  | 15.140 | 11.922 | -6.171  | 1.00 | 13.01 |
| ATOM | 2774 | O   | CYS | 58  | 14.041 | 11.869 | -6.716  | 1.00 | 12.43 |
| ATOM | 2775 | CB  | CYS | 58  | 15.115 | 13.157 | -4.011  | 1.00 | 11.81 |
| ATOM | 2776 | SG  | CYS | 58  | 14.878 | 13.143 | -2.206  | 1.00 | 12.16 |
| ATOM | 2777 | H   | CYS | 58  | 17.254 | 11.786 | -4.000  | 1.00 | 0.00  |
| ATOM | 2778 | N   | VAL | 59  | 16.269 | 12.060 | -6.850  | 1.00 | 13.50 |
| ATOM | 2779 | CA  | VAL | 59  | 16.254 | 12.235 | -8.287  | 1.00 | 15.24 |
| ATOM | 2780 | C   | VAL | 59  | 17.119 | 11.230 | -9.051  | 1.00 | 16.81 |
| ATOM | 2781 | O   | VAL | 59  | 17.322 | 11.381 | -10.255 | 1.00 | 17.91 |
| ATOM | 2782 | CB  | VAL | 59  | 16.652 | 13.692 | -8.653  | 1.00 | 15.93 |
| ATOM | 2783 | CG1 | VAL | 59  | 15.678 | 14.675 | -8.019  | 1.00 | 15.10 |
| ATOM | 2784 | CG2 | VAL | 59  | 18.055 | 14.000 | -8.162  | 1.00 | 16.07 |
| ATOM | 2785 | H   | VAL | 59  | 17.135 | 12.040 | -6.403  | 1.00 | 0.00  |
| ATOM | 2786 | N   | GLY | 60  | 17.565 | 10.171 | -8.377  | 1.00 | 18.29 |
| ATOM | 2787 | CA  | GLY | 60  | 18.400 | 9.171  | -9.027  | 1.00 | 19.78 |
| ATOM | 2788 | C   | GLY | 60  | 18.211 | 7.780  | -8.448  | 1.00 | 21.73 |
| ATOM | 2789 | O   | GLY | 60  | 17.307 | 7.587  | -7.633  | 1.00 | 22.76 |
| ATOM | 2790 | H   | GLY | 60  | 17.367 | 10.069 | -7.421  | 1.00 | 0.00  |
| ATOM | 2791 | N   | PRO | 60A | 19.035 | 6.786  | -8.836  | 1.00 | 22.38 |
| ATOM | 2792 | CA  | PRO | 60A | 20.102 | 6.848  | -9.840  | 1.00 | 23.99 |
| ATOM | 2793 | C   | PRO | 60A | 19.603 | 6.798  | -11.284 | 1.00 | 26.78 |
| ATOM | 2794 | O   | PRO | 60A | 20.330 | 7.160  | -12.211 | 1.00 | 26.72 |
| ATOM | 2795 | CB  | PRO | 60A | 20.949 | 5.627  | -9.499  | 1.00 | 22.26 |
| ATOM | 2796 | CG  | PRO | 60A | 19.927 | 4.652  | -9.071  | 1.00 | 21.97 |
| ATOM | 2797 | CD  | PRO | 60A | 19.061 | 5.483  | -8.153  | 1.00 | 21.93 |
| ATOM | 2798 | N   | ASP | 60B | 18.385 | 6.312  | -11.483 | 1.00 | 29.92 |
| ATOM | 2799 | CA  | ASP | 60B | 17.815 | 6.248  | -12.821 | 1.00 | 32.24 |
| ATOM | 2800 | C   | ASP | 60B | 17.413 | 7.643  | -13.261 | 1.00 | 32.61 |
| ATOM | 2801 | O   | ASP | 60B | 16.755 | 8.369  | -12.508 | 1.00 | 33.74 |
| ATOM | 2802 | CB  | ASP | 60B | 16.625 | 5.295  | -12.852 | 1.00 | 35.70 |
| ATOM | 2803 | CG  | ASP | 60B | 17.052 | 3.843  | -13.013 | 1.00 | 39.63 |
| ATOM | 2804 | OD1 | ASP | 60B | 16.328 | 3.088  | -13.698 | 1.00 | 42.71 |
| ATOM | 2805 | OD2 | ASP | 60B | 18.124 | 3.463  | -12.486 | 1.00 | 39.48 |
| ATOM | 2806 | H   | ASP | 60B | 17.877 | 5.898  | -10.759 | 1.00 | 0.00  |
| ATOM | 2807 | N   | VAL | 60C | 17.825 | 8.010  | -14.471 | 1.00 | 32.19 |
| ATOM | 2808 | CA  | VAL | 60C | 17.566 | 9.328  | -15.042 | 1.00 | 31.81 |
| ATOM | 2809 | C   | VAL | 60C | 16.098 | 9.726  | -15.061 | 1.00 | 32.78 |
| ATOM | 2810 | O   | VAL | 60C | 15.241 | 8.972  | -15.521 | 1.00 | 31.88 |
| ATOM | 2811 | CB  | VAL | 60C | 18.128 | 9.439  | -16.465 | 1.00 | 30.90 |
| ATOM | 2812 | CG1 | VAL | 60C | 17.951 | 10.853 | -16.988 | 1.00 | 31.50 |
| ATOM | 2813 | CG2 | VAL | 60C | 19.585 | 9.053  | -16.480 | 1.00 | 30.47 |
| ATOM | 2814 | H   | VAL | 60C | 18.260 | 7.321  | -14.992 | 1.00 | 0.00  |
| ATOM | 2815 | N   | LYS | 60D | 15.827 | 10.931 | -14.571 | 1.00 | 34.63 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2816 | CA  | LYS | 60D | 14.473 | 11.471 | -14.516 | 1.00 | 36.61 |
| ATOM | 2817 | C   | LYS | 60D | 14.276 | 12.493 | -15.639 | 1.00 | 37.86 |
| ATOM | 2818 | O   | LYS | 60D | 15.255 | 12.944 | -16.248 | 1.00 | 38.80 |
| ATOM | 2819 | CB  | LYS | 60D | 14.231 | 12.134 | -13.156 | 1.00 | 37.46 |
| ATOM | 2820 | CG  | LYS | 60D | 14.432 | 11.209 | -11.958 | 1.00 | 39.46 |
| ATOM | 2821 | CD  | LYS | 60D | 13.524 | 9.976  | -12.021 | 1.00 | 41.12 |
| ATOM | 2822 | CE  | LYS | 60D | 13.587 | 9.147  | -10.743 | 1.00 | 41.39 |
| ATOM | 2823 | NZ  | LYS | 60D | 14.981 | 8.765  | -10.396 | 1.00 | 42.83 |
| ATOM | 2824 | H   | LYS | 60D | 16.579 | 11.494 | -14.309 | 1.00 | 0.00  |
| ATOM | 2825 | HZ1 | LYS | 60D | 15.530 | 9.628  | -10.211 | 1.00 | 0.00  |
| ATOM | 2826 | HZ2 | LYS | 60D | 15.444 | 8.311  | -11.221 | 1.00 | 0.00  |
| ATOM | 2827 | HZ3 | LYS | 60D | 15.003 | 8.161  | -9.553  | 1.00 | 0.00  |
| ATOM | 2828 | N   | ASP | 60E | 13.018 | 12.835 | -15.927 | 1.00 | 37.69 |
| ATOM | 2829 | CA  | ASP | 60E | 12.687 | 13.813 | -16.971 | 1.00 | 36.59 |
| ATOM | 2830 | C   | ASP | 60E | 12.401 | 15.168 | -16.319 | 1.00 | 34.20 |
| ATOM | 2831 | O   | ASP | 60E | 11.424 | 15.321 | -15.585 | 1.00 | 35.05 |
| ATOM | 2832 | CB  | ASP | 60E | 11.468 | 13.344 | -17.780 | 1.00 | 39.68 |
| ATOM | 2833 | CG  | ASP | 60E | 11.082 | 14.316 | -18.901 | 1.00 | 42.67 |
| ATOM | 2834 | OD1 | ASP | 60E | 11.798 | 15.318 | -19.148 | 1.00 | 43.63 |
| ATOM | 2835 | OD2 | ASP | 60E | 10.042 | 14.073 | -19.551 | 1.00 | 44.07 |
| ATOM | 2836 | H   | ASP | 60E | 12.267 | 12.460 | -15.423 | 1.00 | 0.00  |
| ATOM | 2837 | N   | LEU | 61  | 13.233 | 16.157 | -16.628 | 1.00 | 30.70 |
| ATOM | 2838 | CA  | LEU | 61  | 13.104 | 17.495 | -16.058 | 1.00 | 28.24 |
| ATOM | 2839 | C   | LEU | 61  | 11.737 | 18.127 | -16.259 | 1.00 | 27.08 |
| ATOM | 2840 | O   | LEU | 61  | 11.274 | 18.901 | -15.415 | 1.00 | 26.94 |
| ATOM | 2841 | CB  | LEU | 61  | 14.184 | 18.420 | -16.614 | 1.00 | 28.43 |
| ATOM | 2842 | CG  | LEU | 61  | 15.621 | 18.307 | -16.103 | 1.00 | 27.91 |
| ATOM | 2843 | CD1 | LEU | 61  | 16.104 | 16.877 | -16.139 | 1.00 | 28.27 |
| ATOM | 2844 | CD2 | LEU | 61  | 16.511 | 19.182 | -16.968 | 1.00 | 29.59 |
| ATOM | 2845 | H   | LEU | 61  | 13.920 | 15.959 | -17.295 | 1.00 | 0.00  |
| ATOM | 2846 | N   | ALA | 62  | 11.082 | 17.784 | -17.364 | 1.00 | 26.52 |
| ATOM | 2847 | CA  | ALA | 62  | 9.757  | 18.320 | -17.664 | 1.00 | 25.24 |
| ATOM | 2848 | C   | ALA | 62  | 8.742  | 17.859 | -16.616 | 1.00 | 24.34 |
| ATOM | 2849 | O   | ALA | 62  | 7.679  | 18.462 | -16.459 | 1.00 | 24.36 |
| ATOM | 2850 | CB  | ALA | 62  | 9.313  | 17.884 | -19.056 | 1.00 | 23.95 |
| ATOM | 2851 | H   | ALA | 62  | 11.490 | 17.124 | -17.969 | 1.00 | 0.00  |
| ATOM | 2852 | N   | ALA | 63  | 9.076  | 16.779 | -15.917 | 1.00 | 23.30 |
| ATOM | 2853 | CA  | ALA | 63  | 8.213  | 16.212 | -14.891 | 1.00 | 23.20 |
| ATOM | 2854 | C   | ALA | 63  | 8.484  | 16.808 | -13.514 | 1.00 | 22.80 |
| ATOM | 2855 | O   | ALA | 63  | 7.712  | 16.593 | -12.577 | 1.00 | 22.80 |
| ATOM | 2856 | CB  | ALA | 63  | 8.386  | 14.698 | -14.851 | 1.00 | 22.57 |
| ATOM | 2857 | H   | ALA | 63  | 9.919  | 16.312 | -16.072 | 1.00 | 0.00  |
| ATOM | 2858 | N   | LEU | 64  | 9.569  | 17.565 | -13.403 | 1.00 | 22.39 |
| ATOM | 2859 | CA  | LEU | 64  | 9.953  | 18.176 | -12.143 | 1.00 | 23.25 |
| ATOM | 2860 | C   | LEU | 64  | 9.691  | 19.673 | -12.040 | 1.00 | 23.93 |
| ATOM | 2861 | O   | LEU | 64  | 9.748  | 20.421 | -13.029 | 1.00 | 24.43 |
| ATOM | 2862 | CB  | LEU | 64  | 11.432 | 17.929 | -11.854 | 1.00 | 24.96 |
| ATOM | 2863 | CG  | LEU | 64  | 11.853 | 16.614 | -11.213 | 1.00 | 26.97 |
| ATOM | 2864 | CD1 | LEU | 64  | 11.580 | 15.442 | -12.152 | 1.00 | 28.52 |
| ATOM | 2865 | CD2 | LEU | 64  | 13.329 | 16.705 | -10.882 | 1.00 | 26.77 |
| ATOM | 2866 | H   | LEU | 64  | 10.108 | 17.782 | -14.188 | 1.00 | 0.00  |
| ATOM | 2867 | N   | ARG | 65  | 9.471  | 20.104 | -10.805 | 1.00 | 23.23 |
| ATOM | 2868 | CA  | ARG | 65  | 9.219  | 21.493 | -10.474 | 1.00 | 22.50 |
| ATOM | 2869 | C   | ARG | 65  | 9.721  | 21.704 | -9.052  | 1.00 | 22.11 |
| ATOM | 2870 | O   | ARG | 65  | 9.804  | 20.750 | -8.271  | 1.00 | 22.73 |
| ATOM | 2871 | CB  | ARG | 65  | 7.721  | 21.796 | -10.531 | 1.00 | 23.16 |
| ATOM | 2872 | CG  | ARG | 65  | 7.140  | 21.829 | -11.914 | 1.00 | 22.86 |
| ATOM | 2873 | CD  | ARG | 65  | 7.728  | 22.963 | -12.699 | 1.00 | 25.08 |
| ATOM | 2874 | NE  | ARG | 65  | 7.825  | 22.594 | -14.100 | 1.00 | 27.11 |
| ATOM | 2875 | CZ  | ARG | 65  | 6.877  | 22.819 | -14.999 | 1.00 | 27.62 |
| ATOM | 2876 | NH1 | ARG | 65  | 5.749  | 23.428 | -14.643 | 1.00 | 28.46 |
| ATOM | 2877 | NH2 | ARG | 65  | 7.047  | 22.393 | -16.241 | 1.00 | 28.68 |
| ATOM | 2878 | H   | ARG | 65  | 9.476  | 19.442 | -10.080 | 1.00 | 0.00  |

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|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 2879 | HE   | ARG | 65 | 8.651  | 22.085 | -14.311 | 1.00 | 0.00  |
| ATOM | 2880 | HH11 | ARG | 65 | 5.617  | 23.715 | -13.689 | 1.00 | 0.00  |
| ATOM | 2881 | HH12 | ARG | 65 | 5.006  | 23.621 | -15.284 | 1.00 | 0.00  |
| ATOM | 2882 | HH21 | ARG | 65 | 7.879  | 21.881 | -16.479 | 1.00 | 0.00  |
| ATOM | 2883 | HH22 | ARG | 65 | 6.370  | 22.515 | -16.970 | 1.00 | 0.00  |
| ATOM | 2884 | N    | VAL | 66 | 10.043 | 22.953 | -8.728  | 1.00 | 20.10 |
| ATOM | 2885 | CA   | VAL | 66 | 10.530 | 23.338 | -7.409  | 1.00 | 17.28 |
| ATOM | 2886 | C    | VAL | 66 | 9.613  | 24.402 | -6.799  | 1.00 | 17.58 |
| ATOM | 2887 | O    | VAL | 66 | 9.236  | 25.367 | -7.466  | 1.00 | 18.98 |
| ATOM | 2888 | CB   | VAL | 66 | 11.956 | 23.919 | -7.511  | 1.00 | 14.84 |
| ATOM | 2889 | CG1  | VAL | 66 | 12.364 | 24.570 | -6.205  | 1.00 | 14.99 |
| ATOM | 2890 | CG2  | VAL | 66 | 12.933 | 22.825 | -7.878  | 1.00 | 14.12 |
| ATOM | 2891 | H    | VAL | 66 | 9.993  | 23.638 | -9.420  | 1.00 | 0.00  |
| ATOM | 2892 | N    | GLN | 67 | 9.212  | 24.196 | -5.555  | 1.00 | 15.80 |
| ATOM | 2893 | CA   | GLN | 67 | 8.375  | 25.158 | -4.858  | 1.00 | 14.72 |
| ATOM | 2894 | C    | GLN | 67 | 9.218  | 25.660 | -3.724  | 1.00 | 14.29 |
| ATOM | 2895 | O    | GLN | 67 | 9.722  | 24.868 | -2.950  | 1.00 | 16.53 |
| ATOM | 2896 | CB   | GLN | 67 | 7.131  | 24.485 | -4.291  | 1.00 | 14.76 |
| ATOM | 2897 | CG   | GLN | 67 | 6.405  | 25.311 | -3.242  | 1.00 | 16.40 |
| ATOM | 2898 | CD   | GLN | 67 | 5.834  | 26.622 | -3.776  | 1.00 | 19.05 |
| ATOM | 2899 | OE1  | GLN | 67 | 6.067  | 27.011 | -4.924  | 1.00 | 19.16 |
| ATOM | 2900 | NE2  | GLN | 67 | 5.085  | 27.313 | -2.934  | 1.00 | 20.50 |
| ATOM | 2901 | H    | GLN | 67 | 9.454  | 23.368 | -5.096  | 1.00 | 0.00  |
| ATOM | 2902 | HE21 | GLN | 67 | 5.053  | 26.945 | -2.028  | 1.00 | 0.00  |
| ATOM | 2903 | HE22 | GLN | 67 | 4.519  | 28.065 | -3.191  | 1.00 | 0.00  |
| ATOM | 2904 | N    | LEU | 68 | 9.380  | 26.965 | -3.615  | 1.00 | 15.17 |
| ATOM | 2905 | CA   | LEU | 68 | 10.193 | 27.518 | -2.537  | 1.00 | 18.04 |
| ATOM | 2906 | C    | LEU | 68 | 9.415  | 27.477 | -1.221  | 1.00 | 19.10 |
| ATOM | 2907 | O    | LEU | 68 | 8.333  | 26.897 | -1.169  | 1.00 | 20.36 |
| ATOM | 2908 | CB   | LEU | 68 | 10.632 | 28.945 | -2.889  | 1.00 | 19.50 |
| ATOM | 2909 | CG   | LEU | 68 | 11.272 | 29.107 | -4.282  | 1.00 | 21.10 |
| ATOM | 2910 | CD1  | LEU | 68 | 11.599 | 30.560 | -4.562  | 1.00 | 21.08 |
| ATOM | 2911 | CD2  | LEU | 68 | 12.521 | 28.239 | -4.414  | 1.00 | 21.93 |
| ATOM | 2912 | H    | LEU | 68 | 8.938  | 27.552 | -4.261  | 1.00 | 0.00  |
| ATOM | 2913 | N    | ARG | 69 | 9.985  | 28.052 | -0.162  | 1.00 | 20.44 |
| ATOM | 2914 | CA   | ARG | 69 | 9.364  | 28.095 | 1.173   | 1.00 | 21.26 |
| ATOM | 2915 | C    | ARG | 69 | 7.858  | 28.324 | 1.116   | 1.00 | 21.99 |
| ATOM | 2916 | O    | ARG | 69 | 7.398  | 29.319 | 0.559   | 1.00 | 23.44 |
| ATOM | 2917 | CB   | ARG | 69 | 10.009 | 29.204 | 2.007   | 1.00 | 22.01 |
| ATOM | 2918 | CG   | ARG | 69 | 9.411  | 29.425 | 3.395   | 1.00 | 21.35 |
| ATOM | 2919 | CD   | ARG | 69 | 9.821  | 28.351 | 4.375   | 1.00 | 19.91 |
| ATOM | 2920 | NE   | ARG | 69 | 9.553  | 28.744 | 5.757   | 1.00 | 20.69 |
| ATOM | 2921 | CZ   | ARG | 69 | 8.345  | 28.740 | 6.320   | 1.00 | 20.75 |
| ATOM | 2922 | NH1  | ARG | 69 | 7.282  | 28.373 | 5.620   | 1.00 | 20.48 |
| ATOM | 2923 | NH2  | ARG | 69 | 8.196  | 29.057 | 7.598   | 1.00 | 20.48 |
| ATOM | 2924 | H    | ARG | 69 | 10.883 | 28.425 | -0.269  | 1.00 | 0.00  |
| ATOM | 2925 | HE   | ARG | 69 | 10.338 | 29.042 | 6.252   | 1.00 | 0.00  |
| ATOM | 2926 | HH11 | ARG | 69 | 7.358  | 28.083 | 4.667   | 1.00 | 0.00  |
| ATOM | 2927 | HH12 | ARG | 69 | 6.391  | 28.356 | 6.084   | 1.00 | 0.00  |
| ATOM | 2928 | HH21 | ARG | 69 | 8.889  | 29.324 | 8.257   | 1.00 | 0.00  |
| ATOM | 2929 | HH22 | ARG | 69 | 7.266  | 29.001 | 7.985   | 1.00 | 0.00  |
| ATOM | 2930 | N    | GLU | 70 | 7.103  | 27.445 | 1.764   | 1.00 | 21.84 |
| ATOM | 2931 | CA   | GLU | 70 | 5.651  | 27.532 | 1.763   | 1.00 | 22.23 |
| ATOM | 2932 | C    | GLU | 70 | 5.104  | 26.969 | 3.076   | 1.00 | 23.30 |
| ATOM | 2933 | O    | GLU | 70 | 5.443  | 25.846 | 3.452   | 1.00 | 23.20 |
| ATOM | 2934 | CB   | GLU | 70 | 5.139  | 26.719 | 0.576   | 1.00 | 21.53 |
| ATOM | 2935 | CG   | GLU | 70 | 3.662  | 26.816 | 0.277   | 1.00 | 21.77 |
| ATOM | 2936 | CD   | GLU | 70 | 3.311  | 26.073 | -0.996  | 1.00 | 22.44 |
| ATOM | 2937 | OE1  | GLU | 70 | 2.392  | 26.511 | -1.718  | 1.00 | 23.02 |
| ATOM | 2938 | OE2  | GLU | 70 | 3.987  | 25.065 | -1.297  | 1.00 | 22.45 |
| ATOM | 2939 | H    | GLU | 70 | 7.514  | 26.683 | 2.224   | 1.00 | 0.00  |
| ATOM | 2940 | N    | GLN | 71 | 4.300  | 27.754 | 3.795   | 1.00 | 24.46 |
| ATOM | 2941 | CA   | GLN | 71 | 3.733  | 27.296 | 5.073   | 1.00 | 26.04 |

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|------|------|------|-----|----|--------|--------|--------|------|-------|
| ATOM | 2942 | C    | GLN | 71 | 2.814  | 26.089 | 4.968  | 1.00 | 27.48 |
| ATOM | 2943 | O    | GLN | 71 | 2.712  | 25.314 | 5.923  | 1.00 | 29.36 |
| ATOM | 2944 | CB   | GLN | 71 | 2.951  | 28.402 | 5.779  | 1.00 | 26.68 |
| ATOM | 2945 | CG   | GLN | 71 | 3.752  | 29.246 | 6.749  | 1.00 | 28.96 |
| ATOM | 2946 | CD   | GLN | 71 | 4.430  | 28.450 | 7.855  | 1.00 | 28.60 |
| ATOM | 2947 | OE1  | GLN | 71 | 5.638  | 28.574 | 8.048  | 1.00 | 30.20 |
| ATOM | 2948 | NE2  | GLN | 71 | 3.665  | 27.659 | 8.595  | 1.00 | 27.33 |
| ATOM | 2949 | H    | GLN | 71 | 4.068  | 28.640 | 3.448  | 1.00 | 0.00  |
| ATOM | 2950 | HE21 | GLN | 71 | 2.713  | 27.548 | 8.437  | 1.00 | 0.00  |
| ATOM | 2951 | HE22 | GLN | 71 | 4.140  | 27.223 | 9.342  | 1.00 | 0.00  |
| ATOM | 2952 | N    | HIS | 72 | 2.100  | 25.967 | 3.850  | 1.00 | 26.56 |
| ATOM | 2953 | CA   | HIS | 72 | 1.176  | 24.860 | 3.651  | 1.00 | 25.54 |
| ATOM | 2954 | C    | HIS | 72 | 1.350  | 24.268 | 2.259  | 1.00 | 26.53 |
| ATOM | 2955 | O    | HIS | 72 | 1.008  | 24.893 | 1.254  | 1.00 | 26.89 |
| ATOM | 2956 | CB   | HIS | 72 | -0.246 | 25.337 | 3.905  | 1.00 | 24.25 |
| ATOM | 2957 | CG   | HIS | 72 | -0.465 | 25.802 | 5.309  | 1.00 | 24.96 |
| ATOM | 2958 | ND1  | HIS | 72 | -0.510 | 24.935 | 6.379  | 1.00 | 25.83 |
| ATOM | 2959 | CD2  | HIS | 72 | -0.607 | 27.045 | 5.829  | 1.00 | 24.79 |
| ATOM | 2960 | CE1  | HIS | 72 | -0.671 | 25.619 | 7.497  | 1.00 | 25.14 |
| ATOM | 2961 | NE2  | HIS | 72 | -0.733 | 26.902 | 7.190  | 1.00 | 24.96 |
| ATOM | 2962 | H    | HIS | 72 | 2.210  | 26.584 | 3.096  | 1.00 | 0.00  |
| ATOM | 2963 | HD1  | HIS | 72 | -0.410 | 23.963 | 6.263  | 1.00 | 0.00  |
| ATOM | 2964 | HE2  | HIS | 72 | -0.864 | 27.615 | 7.848  | 1.00 | 0.00  |
| ATOM | 2965 | N    | LEU | 73 | 1.809  | 23.018 | 2.242  | 1.00 | 26.03 |
| ATOM | 2966 | CA   | LEU | 73 | 2.134  | 22.267 | 1.030  | 1.00 | 26.58 |
| ATOM | 2967 | C    | LEU | 73 | 1.599  | 22.527 | -0.360 | 1.00 | 27.02 |
| ATOM | 2968 | O    | LEU | 73 | 2.320  | 22.252 | -1.321 | 1.00 | 30.14 |
| ATOM | 2969 | CB   | LEU | 73 | 2.090  | 20.760 | 1.266  | 1.00 | 26.60 |
| ATOM | 2970 | CG   | LEU | 73 | 3.444  | 20.068 | 1.433  | 1.00 | 25.39 |
| ATOM | 2971 | CD1  | LEU | 73 | 3.340  | 18.656 | 0.913  | 1.00 | 25.50 |
| ATOM | 2972 | CD2  | LEU | 73 | 4.535  | 20.811 | 0.687  | 1.00 | 25.01 |
| ATOM | 2973 | H    | LEU | 73 | 1.958  | 22.584 | 3.113  | 1.00 | 0.00  |
| ATOM | 2974 | N    | TYR | 74 | 0.343  | 22.917 | -0.519 | 1.00 | 24.10 |
| ATOM | 2975 | CA   | TYR | 74 | -0.130 | 23.149 | -1.879 | 1.00 | 23.81 |
| ATOM | 2976 | C    | TYR | 74 | -0.955 | 24.408 | -1.978 | 1.00 | 27.06 |
| ATOM | 2977 | O    | TYR | 74 | -1.572 | 24.693 | -3.003 | 1.00 | 26.99 |
| ATOM | 2978 | CB   | TYR | 74 | -0.928 | 21.950 | -2.373 | 1.00 | 20.11 |
| ATOM | 2979 | CG   | TYR | 74 | -0.182 | 20.644 | -2.260 | 1.00 | 17.05 |
| ATOM | 2980 | CD1  | TYR | 74 | -0.371 | 19.809 | -1.162 | 1.00 | 16.55 |
| ATOM | 2981 | CD2  | TYR | 74 | 0.718  | 20.246 | -3.242 | 1.00 | 15.21 |
| ATOM | 2982 | CE1  | TYR | 74 | 0.319  | 18.611 | -1.044 | 1.00 | 15.49 |
| ATOM | 2983 | CE2  | TYR | 74 | 1.411  | 19.053 | -3.134 | 1.00 | 14.58 |
| ATOM | 2984 | CZ   | TYR | 74 | 1.208  | 18.238 | -2.036 | 1.00 | 15.33 |
| ATOM | 2985 | OH   | TYR | 74 | 1.889  | 17.047 | -1.926 | 1.00 | 16.08 |
| ATOM | 2986 | H    | TYR | 74 | -0.229 | 23.081 | 0.248  | 1.00 | 0.00  |
| ATOM | 2987 | HH   | TYR | 74 | 1.801  | 16.700 | -1.028 | 1.00 | 0.00  |
| ATOM | 2988 | N    | TYR | 75 | -0.931 | 25.186 | -0.910 | 1.00 | 31.65 |
| ATOM | 2989 | CA   | TYR | 75 | -1.701 | 26.404 | -0.846 | 1.00 | 36.39 |
| ATOM | 2990 | C    | TYR | 75 | -0.778 | 27.556 | -1.244 | 1.00 | 39.17 |
| ATOM | 2991 | O    | TYR | 75 | 0.125  | 27.939 | -0.495 | 1.00 | 41.04 |
| ATOM | 2992 | CB   | TYR | 75 | -2.295 | 26.557 | 0.568  | 1.00 | 39.44 |
| ATOM | 2993 | CG   | TYR | 75 | -3.060 | 25.311 | 1.049  | 1.00 | 42.68 |
| ATOM | 2994 | CD1  | TYR | 75 | -2.380 | 24.169 | 1.493  | 1.00 | 44.08 |
| ATOM | 2995 | CD2  | TYR | 75 | -4.455 | 25.262 | 1.028  | 1.00 | 43.19 |
| ATOM | 2996 | CE1  | TYR | 75 | -3.073 | 23.015 | 1.898  | 1.00 | 43.78 |
| ATOM | 2997 | CE2  | TYR | 75 | -5.153 | 24.109 | 1.433  | 1.00 | 43.52 |
| ATOM | 2998 | CZ   | TYR | 75 | -4.455 | 22.994 | 1.866  | 1.00 | 43.62 |
| ATOM | 2999 | OH   | TYR | 75 | -5.137 | 21.864 | 2.268  | 1.00 | 43.43 |
| ATOM | 3000 | H    | TYR | 75 | -0.265 | 25.020 | -0.212 | 1.00 | 0.00  |
| ATOM | 3001 | HH   | TYR | 75 | -6.095 | 22.027 | 2.259  | 1.00 | 0.00  |
| ATOM | 3002 | N    | GLN | 79 | -1.011 | 28.062 | -2.454 | 1.00 | 40.20 |
| ATOM | 3003 | CA   | GLN | 79 | -0.256 | 29.155 | -3.079 | 1.00 | 40.33 |
| ATOM | 3004 | C    | GLN | 79 | 0.962  | 28.596 | -3.789 | 1.00 | 37.64 |

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|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 3005 | O    | GLN | 79 | 2.074  | 29.115 | -3.683  | 1.00 | 36.67 |
| ATOM | 3006 | CB   | GLN | 79 | 0.124  | 30.271 | -2.086  | 1.00 | 45.26 |
| ATOM | 3007 | CG   | GLN | 79 | 0.853  | 31.509 | -2.704  | 1.00 | 51.67 |
| ATOM | 3008 | CD   | GLN | 79 | 0.066  | 32.239 | -3.813  | 1.00 | 54.23 |
| ATOM | 3009 | OE1  | GLN | 79 | -1.125 | 32.540 | -3.664  | 1.00 | 55.60 |
| ATOM | 3010 | NE2  | GLN | 79 | 0.750  | 32.553 | -4.913  | 1.00 | 53.74 |
| ATOM | 3011 | H    | GLN | 79 | -1.717 | 27.635 | -2.978  | 1.00 | 0.00  |
| ATOM | 3012 | HE21 | GLN | 79 | 1.706  | 32.319 | -4.951  | 1.00 | 0.00  |
| ATOM | 3013 | HE22 | GLN | 79 | 0.269  | 33.003 | -5.631  | 1.00 | 0.00  |
| ATOM | 3014 | N    | ASP | 80 | 0.730  | 27.512 | -4.514  | 1.00 | 35.38 |
| ATOM | 3015 | CA   | ASP | 80 | 1.781  | 26.876 | -5.280  | 1.00 | 33.84 |
| ATOM | 3016 | C    | ASP | 80 | 2.280  | 27.868 | -6.316  | 1.00 | 33.21 |
| ATOM | 3017 | O    | ASP | 80 | 1.506  | 28.658 | -6.853  | 1.00 | 33.16 |
| ATOM | 3018 | CB   | ASP | 80 | 1.236  | 25.644 | -6.000  | 1.00 | 33.14 |
| ATOM | 3019 | CG   | ASP | 80 | 1.616  | 24.352 | -5.318  | 1.00 | 31.13 |
| ATOM | 3020 | OD1  | ASP | 80 | 2.074  | 24.394 | -4.160  | 1.00 | 30.14 |
| ATOM | 3021 | OD2  | ASP | 80 | 1.468  | 23.286 | -5.952  | 1.00 | 29.87 |
| ATOM | 3022 | H    | ASP | 80 | -0.147 | 27.096 | -4.508  | 1.00 | 0.00  |
| ATOM | 3023 | N    | GLN | 81 | 3.575  | 27.812 | -6.592  | 1.00 | 33.02 |
| ATOM | 3024 | CA   | GLN | 81 | 4.220  | 28.675 | -7.572  | 1.00 | 32.15 |
| ATOM | 3025 | C    | GLN | 81 | 5.454  | 27.907 | -8.035  | 1.00 | 29.69 |
| ATOM | 3026 | O    | GLN | 81 | 6.595  | 28.306 | -7.801  | 1.00 | 29.42 |
| ATOM | 3027 | CB   | GLN | 81 | 4.586  | 30.018 | -6.935  | 1.00 | 35.77 |
| ATOM | 3028 | CG   | GLN | 81 | 5.297  | 29.901 | -5.590  | 1.00 | 41.85 |
| ATOM | 3029 | CD   | GLN | 81 | 4.686  | 30.786 | -4.505  | 1.00 | 45.18 |
| ATOM | 3030 | OE1  | GLN | 81 | 4.149  | 31.867 | -4.783  | 1.00 | 45.71 |
| ATOM | 3031 | NE2  | GLN | 81 | 4.769  | 30.326 | -3.257  | 1.00 | 45.70 |
| ATOM | 3032 | H    | GLN | 81 | 4.122  | 27.157 | -6.102  | 1.00 | 0.00  |
| ATOM | 3033 | HE21 | GLN | 81 | 5.209  | 29.474 | -3.068  | 1.00 | 0.00  |
| ATOM | 3034 | HE22 | GLN | 81 | 4.349  | 30.887 | -2.576  | 1.00 | 0.00  |
| ATOM | 3035 | N    | LEU | 82 | 5.192  | 26.765 | -8.661  | 1.00 | 26.81 |
| ATOM | 3036 | CA   | LEU | 82 | 6.225  | 25.864 | -9.158  | 1.00 | 24.87 |
| ATOM | 3037 | C    | LEU | 82 | 7.261  | 26.524 | -10.070 | 1.00 | 24.59 |
| ATOM | 3038 | O    | LEU | 82 | 6.938  | 27.426 | -10.837 | 1.00 | 26.38 |
| ATOM | 3039 | CB   | LEU | 82 | 5.579  | 24.674 | -9.881  | 1.00 | 21.39 |
| ATOM | 3040 | CG   | LEU | 82 | 4.519  | 23.854 | -9.139  | 1.00 | 18.22 |
| ATOM | 3041 | CD1  | LEU | 82 | 4.728  | 23.958 | -7.647  | 1.00 | 18.78 |
| ATOM | 3042 | CD2  | LEU | 82 | 3.134  | 24.336 | -9.488  | 1.00 | 20.24 |
| ATOM | 3043 | H    | LEU | 82 | 4.250  | 26.550 | -8.792  | 1.00 | 0.00  |
| ATOM | 3044 | N    | LEU | 83 | 8.504  | 26.067 | -9.981  | 1.00 | 22.76 |
| ATOM | 3045 | CA   | LEU | 83 | 9.577  | 26.605 | -10.799 | 1.00 | 22.62 |
| ATOM | 3046 | C    | LEU | 83 | 10.222 | 25.495 | -11.621 | 1.00 | 24.07 |
| ATOM | 3047 | O    | LEU | 83 | 10.481 | 24.402 | -11.107 | 1.00 | 23.84 |
| ATOM | 3048 | CB   | LEU | 83 | 10.640 | 27.258 | -9.919  | 1.00 | 21.97 |
| ATOM | 3049 | CG   | LEU | 83 | 10.183 | 28.361 | -8.970  | 1.00 | 22.43 |
| ATOM | 3050 | CD1  | LEU | 83 | 11.392 | 29.007 | -8.320  | 1.00 | 22.99 |
| ATOM | 3051 | CD2  | LEU | 83 | 9.388  | 29.397 | -9.730  | 1.00 | 24.38 |
| ATOM | 3052 | H    | LEU | 83 | 8.716  | 25.397 | -9.304  | 1.00 | 0.00  |
| ATOM | 3053 | N    | PRO | 84 | 10.445 | 25.739 | -12.923 | 1.00 | 24.83 |
| ATOM | 3054 | CA   | PRO | 84 | 11.064 | 24.737 | -13.788 | 1.00 | 25.04 |
| ATOM | 3055 | C    | PRO | 84 | 12.568 | 24.606 | -13.539 | 1.00 | 26.70 |
| ATOM | 3056 | O    | PRO | 84 | 13.240 | 25.567 | -13.143 | 1.00 | 26.43 |
| ATOM | 3057 | CB   | PRO | 84 | 10.771 | 25.273 | -15.183 | 1.00 | 24.05 |
| ATOM | 3058 | CG   | PRO | 84 | 10.820 | 26.734 | -14.987 | 1.00 | 24.45 |
| ATOM | 3059 | CD   | PRO | 84 | 10.036 | 26.914 | -13.711 | 1.00 | 25.04 |
| ATOM | 3060 | N    | VAL | 85 | 13.069 | 23.395 | -13.763 | 1.00 | 27.88 |
| ATOM | 3061 | CA   | VAL | 85 | 14.474 | 23.050 | -13.597 | 1.00 | 26.80 |
| ATOM | 3062 | C    | VAL | 85 | 15.106 | 22.978 | -14.981 | 1.00 | 27.62 |
| ATOM | 3063 | O    | VAL | 85 | 14.478 | 22.512 | -15.931 | 1.00 | 29.02 |
| ATOM | 3064 | CB   | VAL | 85 | 14.603 | 21.677 | -12.927 | 1.00 | 25.93 |
| ATOM | 3065 | CG1  | VAL | 85 | 16.045 | 21.216 | -12.923 | 1.00 | 26.71 |
| ATOM | 3066 | CG2  | VAL | 85 | 14.057 | 21.743 | -11.517 | 1.00 | 27.01 |
| ATOM | 3067 | H    | VAL | 85 | 12.479 | 22.686 | -14.091 | 1.00 | 0.00  |

|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 3068 | N    | SER | 86 | 16.357 | 23.401 | -15.089 | 1.00 | 27.09 |
| ATOM | 3069 | CA   | SER | 86 | 17.052 | 23.383 | -16.365 | 1.00 | 26.70 |
| ATOM | 3070 | C    | SER | 86 | 18.112 | 22.297 | -16.434 | 1.00 | 26.19 |
| ATOM | 3071 | O    | SER | 86 | 18.439 | 21.788 | -17.516 | 1.00 | 27.64 |
| ATOM | 3072 | CB   | SER | 86 | 17.690 | 24.743 | -16.619 | 1.00 | 27.96 |
| ATOM | 3073 | OG   | SER | 86 | 18.409 | 25.162 | -15.478 | 1.00 | 30.97 |
| ATOM | 3074 | H    | SER | 86 | 16.834 | 23.716 | -14.302 | 1.00 | 0.00  |
| ATOM | 3075 | HG   | SER | 86 | 18.180 | 26.055 | -15.190 | 1.00 | 0.00  |
| ATOM | 3076 | N    | ARG | 87 | 18.625 | 21.900 | -15.281 | 1.00 | 24.37 |
| ATOM | 3077 | CA   | ARG | 87 | 19.661 | 20.893 | -15.286 | 1.00 | 23.98 |
| ATOM | 3078 | C    | ARG | 87 | 19.688 | 20.201 | -13.942 | 1.00 | 21.85 |
| ATOM | 3079 | O    | ARG | 87 | 19.490 | 20.841 | -12.912 | 1.00 | 21.59 |
| ATOM | 3080 | CB   | ARG | 87 | 20.990 | 21.593 | -15.587 | 1.00 | 26.89 |
| ATOM | 3081 | CG   | ARG | 87 | 22.136 | 20.709 | -16.036 | 1.00 | 29.45 |
| ATOM | 3082 | CD   | ARG | 87 | 23.149 | 21.515 | -16.846 | 1.00 | 29.90 |
| ATOM | 3083 | NE   | ARG | 87 | 23.399 | 22.830 | -16.267 | 1.00 | 30.32 |
| ATOM | 3084 | CZ   | ARG | 87 | 24.595 | 23.284 | -15.904 | 1.00 | 30.98 |
| ATOM | 3085 | NH1  | ARG | 87 | 25.672 | 22.524 | -16.059 | 1.00 | 30.98 |
| ATOM | 3086 | NH2  | ARG | 87 | 24.707 | 24.499 | -15.372 | 1.00 | 30.47 |
| ATOM | 3087 | H    | ARG | 87 | 18.353 | 22.309 | -14.434 | 1.00 | 0.00  |
| ATOM | 3088 | HE   | ARG | 87 | 22.628 | 23.433 | -16.122 | 1.00 | 0.00  |
| ATOM | 3089 | HH11 | ARG | 87 | 25.618 | 21.608 | -16.475 | 1.00 | 0.00  |
| ATOM | 3090 | HH12 | ARG | 87 | 26.589 | 22.864 | -15.797 | 1.00 | 0.00  |
| ATOM | 3091 | HH21 | ARG | 87 | 23.869 | 25.063 | -15.222 | 1.00 | 0.00  |
| ATOM | 3092 | HH22 | ARG | 87 | 25.564 | 24.907 | -15.064 | 1.00 | 0.00  |
| ATOM | 3093 | N    | ILE | 88 | 19.850 | 18.884 | -13.969 | 1.00 | 20.50 |
| ATOM | 3094 | CA   | ILE | 88 | 19.913 | 18.066 | -12.759 | 1.00 | 22.18 |
| ATOM | 3095 | C    | ILE | 88 | 21.308 | 17.445 | -12.703 | 1.00 | 23.46 |
| ATOM | 3096 | O    | ILE | 88 | 21.732 | 16.771 | -13.644 | 1.00 | 24.82 |
| ATOM | 3097 | CB   | ILE | 88 | 18.859 | 16.913 | -12.780 | 1.00 | 22.63 |
| ATOM | 3098 | CG1  | ILE | 88 | 17.438 | 17.481 | -12.817 | 1.00 | 23.16 |
| ATOM | 3099 | CG2  | ILE | 88 | 19.027 | 15.995 | -11.572 | 1.00 | 20.50 |
| ATOM | 3100 | H    | ILE | 88 | 19.953 | 18.439 | -14.842 | 1.00 | 0.00  |
| ATOM | 3101 | CD   | ILE | 88 | 16.370 | 16.419 | -12.796 | 1.00 | 24.85 |
| ATOM | 3102 | N    | ILE | 89 | 22.032 | 17.687 | -11.620 | 1.00 | 23.34 |
| ATOM | 3103 | CA   | ILE | 89 | 23.373 | 17.139 | -11.481 | 1.00 | 22.63 |
| ATOM | 3104 | C    | ILE | 89 | 23.463 | 16.186 | -10.300 | 1.00 | 22.23 |
| ATOM | 3105 | O    | ILE | 89 | 23.388 | 16.596 | -9.140  | 1.00 | 22.16 |
| ATOM | 3106 | CB   | ILE | 89 | 24.425 | 18.255 | -11.399 | 1.00 | 22.65 |
| ATOM | 3107 | CG1  | ILE | 89 | 24.535 | 18.926 | -12.769 | 1.00 | 22.29 |
| ATOM | 3108 | CG2  | ILE | 89 | 25.770 | 17.695 | -10.969 | 1.00 | 22.49 |
| ATOM | 3109 | H    | ILE | 89 | 21.661 | 18.228 | -10.916 | 1.00 | 0.00  |
| ATOM | 3110 | CD   | ILE | 89 | 25.457 | 20.087 | -12.806 | 1.00 | 25.72 |
| ATOM | 3111 | N    | VAL | 90 | 23.561 | 14.901 | -10.629 | 1.00 | 21.11 |
| ATOM | 3112 | CA   | VAL | 90 | 23.642 | 13.825 | -9.652  | 1.00 | 18.37 |
| ATOM | 3113 | C    | VAL | 90 | 25.093 | 13.402 | -9.491  | 1.00 | 16.51 |
| ATOM | 3114 | O    | VAL | 90 | 25.788 | 13.168 | -10.480 | 1.00 | 14.67 |
| ATOM | 3115 | CB   | VAL | 90 | 22.807 | 12.613 | -10.112 | 1.00 | 17.30 |
| ATOM | 3116 | CG1  | VAL | 90 | 22.950 | 11.458 | -9.139  | 1.00 | 19.21 |
| ATOM | 3117 | CG2  | VAL | 90 | 21.356 | 13.007 | -10.240 | 1.00 | 17.04 |
| ATOM | 3118 | H    | VAL | 90 | 23.611 | 14.677 | -11.581 | 1.00 | 0.00  |
| ATOM | 3119 | N    | HIS | 91 | 25.550 | 13.323 | -8.245  | 1.00 | 14.91 |
| ATOM | 3120 | CA   | HIS | 91 | 26.912 | 12.927 | -7.984  | 1.00 | 14.56 |
| ATOM | 3121 | C    | HIS | 91 | 27.140 | 11.568 | -8.620  | 1.00 | 16.19 |
| ATOM | 3122 | O    | HIS | 91 | 26.495 | 10.587 | -8.261  | 1.00 | 17.08 |
| ATOM | 3123 | CB   | HIS | 91 | 27.180 | 12.852 | -6.491  | 1.00 | 14.24 |
| ATOM | 3124 | CG   | HIS | 91 | 28.632 | 12.716 | -6.158  | 1.00 | 13.82 |
| ATOM | 3125 | ND1  | HIS | 91 | 29.425 | 13.794 | -5.824  | 1.00 | 14.00 |
| ATOM | 3126 | CD2  | HIS | 91 | 29.446 | 11.635 | -6.144  | 1.00 | 12.66 |
| ATOM | 3127 | CE1  | HIS | 91 | 30.661 | 13.384 | -5.618  | 1.00 | 12.98 |
| ATOM | 3128 | NE2  | HIS | 91 | 30.700 | 12.078 | -5.807  | 1.00 | 13.51 |
| ATOM | 3129 | H    | HIS | 91 | 24.957 | 13.508 | -7.484  | 1.00 | 0.00  |
| ATOM | 3130 | HD1  | HIS | 91 | 29.117 | 14.726 | -5.748  | 1.00 | 0.00  |

|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 3131 | HE2  | HIS | 91 | 31.515 | 11.538 | -5.714  | 1.00 | 0.00  |
| ATOM | 3132 | N    | PRO | 92 | 28.130 | 11.478 | -9.513  | 1.00 | 17.82 |
| ATOM | 3133 | CA   | PRO | 92 | 28.496 | 10.255 | -10.239 | 1.00 | 17.81 |
| ATOM | 3134 | C    | PRO | 92 | 28.666 | 8.970  | -9.442  | 1.00 | 17.65 |
| ATOM | 3135 | O    | PRO | 92 | 28.420 | 7.893  | -9.970  | 1.00 | 19.34 |
| ATOM | 3136 | CB   | PRO | 92 | 29.791 | 10.648 | -10.956 | 1.00 | 17.26 |
| ATOM | 3137 | CG   | PRO | 92 | 30.326 | 11.790 | -10.127 | 1.00 | 18.76 |
| ATOM | 3138 | CD   | PRO | 92 | 29.086 | 12.560 | -9.803  | 1.00 | 18.30 |
| ATOM | 3139 | N    | GLN | 93 | 29.092 | 9.065  | -8.190  | 1.00 | 17.14 |
| ATOM | 3140 | CA   | GLN | 93 | 29.292 | 7.863  | -7.392  | 1.00 | 18.42 |
| ATOM | 3141 | C    | GLN | 93 | 28.035 | 7.359  | -6.739  | 1.00 | 18.03 |
| ATOM | 3142 | O    | GLN | 93 | 28.070 | 6.372  | -6.005  | 1.00 | 19.16 |
| ATOM | 3143 | CB   | GLN | 93 | 30.350 | 8.084  | -6.318  | 1.00 | 22.02 |
| ATOM | 3144 | CG   | GLN | 93 | 31.728 | 8.382  | -6.864  | 1.00 | 28.17 |
| ATOM | 3145 | CD   | GLN | 93 | 32.828 | 7.919  | -5.935  | 1.00 | 31.41 |
| ATOM | 3146 | OE1  | GLN | 93 | 33.531 | 6.946  | -6.227  | 1.00 | 33.61 |
| ATOM | 3147 | NE2  | GLN | 93 | 32.981 | 8.605  | -4.804  | 1.00 | 32.92 |
| ATOM | 3148 | H    | GLN | 93 | 29.242 | 9.942  | -7.818  | 1.00 | 0.00  |
| ATOM | 3149 | HE21 | GLN | 93 | 32.406 | 9.350  | -4.576  | 1.00 | 0.00  |
| ATOM | 3150 | HE22 | GLN | 93 | 33.719 | 8.285  | -4.245  | 1.00 | 0.00  |
| ATOM | 3151 | N    | PHE | 94 | 26.922 | 8.030  | -6.995  | 1.00 | 17.80 |
| ATOM | 3152 | CA   | PHE | 94 | 25.674 | 7.621  | -6.389  | 1.00 | 17.79 |
| ATOM | 3153 | C    | PHE | 94 | 24.954 | 6.511  | -7.102  | 1.00 | 17.90 |
| ATOM | 3154 | O    | PHE | 94 | 24.847 | 6.509  | -8.322  | 1.00 | 19.86 |
| ATOM | 3155 | CB   | PHE | 94 | 24.700 | 8.786  | -6.259  | 1.00 | 18.50 |
| ATOM | 3156 | CG   | PHE | 94 | 23.375 | 8.384  | -5.676  | 1.00 | 20.01 |
| ATOM | 3157 | CD1  | PHE | 94 | 23.276 | 8.011  | -4.336  | 1.00 | 20.50 |
| ATOM | 3158 | CD2  | PHE | 94 | 22.238 | 8.316  | -6.472  | 1.00 | 21.38 |
| ATOM | 3159 | CE1  | PHE | 94 | 22.073 | 7.571  | -3.803  | 1.00 | 19.68 |
| ATOM | 3160 | CE2  | PHE | 94 | 21.025 | 7.876  | -5.942  | 1.00 | 21.21 |
| ATOM | 3161 | CZ   | PHE | 94 | 20.949 | 7.504  | -4.606  | 1.00 | 20.25 |
| ATOM | 3162 | H    | PHE | 94 | 26.870 | 8.777  | -7.617  | 1.00 | 0.00  |
| ATOM | 3163 | N    | TYR | 95 | 24.429 | 5.587  | -6.312  | 1.00 | 18.03 |
| ATOM | 3164 | CA   | TYR | 95 | 23.629 | 4.479  | -6.813  | 1.00 | 18.49 |
| ATOM | 3165 | C    | TYR | 95 | 22.711 | 3.996  | -5.689  | 1.00 | 17.84 |
| ATOM | 3166 | O    | TYR | 95 | 21.598 | 3.548  | -5.936  | 1.00 | 19.19 |
| ATOM | 3167 | CB   | TYR | 95 | 24.473 | 3.310  | -7.346  | 1.00 | 20.03 |
| ATOM | 3168 | CG   | TYR | 95 | 23.590 | 2.189  | -7.867  | 1.00 | 22.55 |
| ATOM | 3169 | CD1  | TYR | 95 | 22.914 | 2.313  | -9.086  | 1.00 | 23.53 |
| ATOM | 3170 | CD2  | TYR | 95 | 23.324 | 1.063  | -7.085  | 1.00 | 22.97 |
| ATOM | 3171 | CE1  | TYR | 95 | 21.986 | 1.352  | -9.506  | 1.00 | 23.67 |
| ATOM | 3172 | CE2  | TYR | 95 | 22.397 | 0.098  | -7.495  | 1.00 | 23.89 |
| ATOM | 3173 | CZ   | TYR | 95 | 21.730 | 0.251  | -8.702  | 1.00 | 24.25 |
| ATOM | 3174 | OH   | TYR | 95 | 20.796 | -0.688 | -9.082  | 1.00 | 25.15 |
| ATOM | 3175 | H    | TYR | 95 | 24.612 | 5.705  | -5.360  | 1.00 | 0.00  |
| ATOM | 3176 | HH   | TYR | 95 | 20.347 | -0.398 | -9.893  | 1.00 | 0.00  |
| ATOM | 3177 | N    | THR | 96 | 23.174 | 4.120  | -4.451  | 1.00 | 16.68 |
| ATOM | 3178 | CA   | THR | 96 | 22.410 | 3.696  | -3.289  | 1.00 | 14.87 |
| ATOM | 3179 | C    | THR | 96 | 22.768 | 4.584  | -2.106  | 1.00 | 15.76 |
| ATOM | 3180 | O    | THR | 96 | 23.901 | 5.050  | -1.991  | 1.00 | 16.26 |
| ATOM | 3181 | CB   | THR | 96 | 22.732 | 2.229  | -2.947  | 1.00 | 14.73 |
| ATOM | 3182 | OG1  | THR | 96 | 21.909 | 1.357  | -3.725  | 1.00 | 16.07 |
| ATOM | 3183 | CG2  | THR | 96 | 22.526 | 1.948  | -1.499  | 1.00 | 14.86 |
| ATOM | 3184 | H    | THR | 96 | 24.069 | 4.484  | -4.291  | 1.00 | 0.00  |
| ATOM | 3185 | HG1  | THR | 96 | 20.987 | 1.624  | -3.669  | 1.00 | 0.00  |
| ATOM | 3186 | N    | ALA | 97 | 21.799 | 4.816  | -1.229  | 1.00 | 16.38 |
| ATOM | 3187 | CA   | ALA | 97 | 22.018 | 5.638  | -0.048  | 1.00 | 16.61 |
| ATOM | 3188 | C    | ALA | 97 | 23.063 | 5.003  | 0.871   | 1.00 | 18.45 |
| ATOM | 3189 | O    | ALA | 97 | 24.058 | 5.629  | 1.208   | 1.00 | 20.27 |
| ATOM | 3190 | CB   | ALA | 97 | 20.715 | 5.828  | 0.698   | 1.00 | 16.35 |
| ATOM | 3191 | H    | ALA | 97 | 20.919 | 4.418  | -1.380  | 1.00 | 0.00  |
| ATOM | 3192 | N    | GLN | 98 | 22.862 | 3.734  | 1.220   | 1.00 | 20.21 |
| ATOM | 3193 | CA   | GLN | 98 | 23.764 | 2.996  | 2.117   | 1.00 | 21.87 |

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|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3194 | C    | GLN | 98  | 25.193 | 2.980  | 1.597  | 1.00 | 20.81 |
| ATOM | 3195 | O    | GLN | 98  | 26.151 | 2.835  | 2.361  | 1.00 | 19.93 |
| ATOM | 3196 | CB   | GLN | 98  | 23.295 | 1.544  | 2.297  | 1.00 | 24.44 |
| ATOM | 3197 | CG   | GLN | 98  | 21.982 | 1.371  | 3.035  | 1.00 | 27.69 |
| ATOM | 3198 | CD   | GLN | 98  | 20.818 | 2.007  | 2.311  | 1.00 | 30.78 |
| ATOM | 3199 | OE1  | GLN | 98  | 20.808 | 2.094  | 1.084  | 1.00 | 31.89 |
| ATOM | 3200 | NE2  | GLN | 98  | 19.836 | 2.476  | 3.066  | 1.00 | 33.22 |
| ATOM | 3201 | H    | GLN | 98  | 22.113 | 3.291  | 0.794  | 1.00 | 0.00  |
| ATOM | 3202 | HE21 | GLN | 98  | 19.928 | 2.360  | 4.032  | 1.00 | 0.00  |
| ATOM | 3203 | HE22 | GLN | 98  | 19.073 | 2.895  | 2.610  | 1.00 | 0.00  |
| ATOM | 3204 | N    | ILE | 99  | 25.317 | 3.046  | 0.280  | 1.00 | 20.30 |
| ATOM | 3205 | CA   | ILE | 99  | 26.611 | 3.052  | -0.358 | 1.00 | 21.90 |
| ATOM | 3206 | C    | ILE | 99  | 27.280 | 4.406  | -0.124 | 1.00 | 23.75 |
| ATOM | 3207 | O    | ILE | 99  | 28.421 | 4.453  | 0.332  | 1.00 | 26.39 |
| ATOM | 3208 | CB   | ILE | 99  | 26.480 | 2.689  | -1.850 | 1.00 | 21.91 |
| ATOM | 3209 | CG1  | ILE | 99  | 26.382 | 1.166  | -1.985 | 1.00 | 21.54 |
| ATOM | 3210 | CG2  | ILE | 99  | 27.633 | 3.255  | -2.653 | 1.00 | 24.65 |
| ATOM | 3211 | H    | ILE | 99  | 24.518 | 3.118  | -0.269 | 1.00 | 0.00  |
| ATOM | 3212 | CD   | ILE | 99  | 26.231 | 0.657  | -3.394 | 1.00 | 19.95 |
| ATOM | 3213 | N    | GLY | 100 | 26.570 | 5.498  | -0.401 | 1.00 | 23.83 |
| ATOM | 3214 | CA   | GLY | 100 | 27.129 | 6.822  | -0.174 | 1.00 | 21.64 |
| ATOM | 3215 | C    | GLY | 100 | 26.976 | 7.786  | -1.333 | 1.00 | 20.52 |
| ATOM | 3216 | O    | GLY | 100 | 26.308 | 7.494  | -2.325 | 1.00 | 19.73 |
| ATOM | 3217 | H    | GLY | 100 | 25.683 | 5.438  | -0.817 | 1.00 | 0.00  |
| ATOM | 3218 | N    | ALA | 101 | 27.577 | 8.960  | -1.186 | 1.00 | 20.72 |
| ATOM | 3219 | CA   | ALA | 101 | 27.542 | 9.994  | -2.211 | 1.00 | 20.27 |
| ATOM | 3220 | C    | ALA | 101 | 26.154 | 10.540 | -2.481 | 1.00 | 19.41 |
| ATOM | 3221 | O    | ALA | 101 | 25.931 | 11.192 | -3.496 | 1.00 | 21.65 |
| ATOM | 3222 | CB   | ALA | 101 | 28.158 | 9.477  | -3.505 | 1.00 | 19.99 |
| ATOM | 3223 | H    | ALA | 101 | 28.094 | 9.152  | -0.370 | 1.00 | 0.00  |
| ATOM | 3224 | N    | ASP | 102 | 25.240 | 10.343 | -1.544 | 1.00 | 17.49 |
| ATOM | 3225 | CA   | ASP | 102 | 23.873 | 10.806 | -1.724 | 1.00 | 15.51 |
| ATOM | 3226 | C    | ASP | 102 | 23.738 | 12.320 | -1.696 | 1.00 | 15.17 |
| ATOM | 3227 | O    | ASP | 102 | 23.385 | 12.902 | -0.676 | 1.00 | 15.11 |
| ATOM | 3228 | CB   | ASP | 102 | 22.974 | 10.197 | -0.660 | 1.00 | 15.37 |
| ATOM | 3229 | CG   | ASP | 102 | 21.526 | 10.219 | -1.048 | 1.00 | 16.45 |
| ATOM | 3230 | OD1  | ASP | 102 | 21.174 | 10.789 | -2.096 | 1.00 | 16.31 |
| ATOM | 3231 | OD2  | ASP | 102 | 20.719 | 9.642  | -0.306 | 1.00 | 19.62 |
| ATOM | 3232 | H    | ASP | 102 | 25.491 | 9.899  | -0.710 | 1.00 | 0.00  |
| ATOM | 3233 | N    | ILE | 103 | 23.992 | 12.957 | -2.829 | 1.00 | 14.64 |
| ATOM | 3234 | CA   | ILE | 103 | 23.890 | 14.404 | -2.921 | 1.00 | 14.84 |
| ATOM | 3235 | C    | ILE | 103 | 23.626 | 14.746 | -4.389 | 1.00 | 15.54 |
| ATOM | 3236 | O    | ILE | 103 | 24.140 | 14.065 | -5.292 | 1.00 | 15.63 |
| ATOM | 3237 | CB   | ILE | 103 | 25.195 | 15.082 | -2.384 | 1.00 | 15.38 |
| ATOM | 3238 | CG1  | ILE | 103 | 24.935 | 16.540 | -1.988 | 1.00 | 14.76 |
| ATOM | 3239 | CG2  | ILE | 103 | 26.327 | 14.967 | -3.404 | 1.00 | 14.78 |
| ATOM | 3240 | H    | ILE | 103 | 24.286 | 12.439 | -3.609 | 1.00 | 0.00  |
| ATOM | 3241 | CD   | ILE | 103 | 26.094 | 17.201 | -1.268 | 1.00 | 11.34 |
| ATOM | 3242 | N    | ALA | 104 | 22.785 | 15.753 | -4.623 | 1.00 | 15.37 |
| ATOM | 3243 | CA   | ALA | 104 | 22.428 | 16.178 | -5.976 | 1.00 | 15.05 |
| ATOM | 3244 | C    | ALA | 104 | 22.124 | 17.660 | -6.019 | 1.00 | 15.32 |
| ATOM | 3245 | O    | ALA | 104 | 21.809 | 18.263 | -4.996 | 1.00 | 16.76 |
| ATOM | 3246 | CB   | ALA | 104 | 21.236 | 15.399 | -6.472 | 1.00 | 15.24 |
| ATOM | 3247 | H    | ALA | 104 | 22.358 | 16.234 | -3.890 | 1.00 | 0.00  |
| ATOM | 3248 | N    | LEU | 105 | 22.200 | 18.228 | -7.215 | 1.00 | 15.71 |
| ATOM | 3249 | CA   | LEU | 105 | 21.960 | 19.646 | -7.442 | 1.00 | 17.31 |
| ATOM | 3250 | C    | LEU | 105 | 20.948 | 19.862 | -8.561 | 1.00 | 19.06 |
| ATOM | 3251 | O    | LEU | 105 | 21.033 | 19.222 | -9.611 | 1.00 | 19.06 |
| ATOM | 3252 | CB   | LEU | 105 | 23.262 | 20.328 | -7.868 | 1.00 | 17.05 |
| ATOM | 3253 | CG   | LEU | 105 | 24.444 | 20.403 | -6.910 | 1.00 | 16.15 |
| ATOM | 3254 | CD1  | LEU | 105 | 25.683 | 20.853 | -7.669 | 1.00 | 15.03 |
| ATOM | 3255 | CD2  | LEU | 105 | 24.113 | 21.362 | -5.777 | 1.00 | 16.80 |
| ATOM | 3256 | H    | LEU | 105 | 22.468 | 17.677 | -7.971 | 1.00 | 0.00  |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 3257 | N   | LEU | 106 | 20.015 | 20.784 | -8.354  | 1.00 | 18.81 |
| ATOM | 3258 | CA  | LEU | 106 | 19.022 | 21.095 | -9.369  | 1.00 | 18.38 |
| ATOM | 3259 | C   | LEU | 106 | 19.249 | 22.552 | -9.721  | 1.00 | 19.95 |
| ATOM | 3260 | O   | LEU | 106 | 19.358 | 23.389 | -8.827  | 1.00 | 20.25 |
| ATOM | 3261 | CB  | LEU | 106 | 17.613 | 20.923 | -8.818  | 1.00 | 18.45 |
| ATOM | 3262 | CG  | LEU | 106 | 17.302 | 19.714 | -7.932  | 1.00 | 19.10 |
| ATOM | 3263 | CD1 | LEU | 106 | 15.795 | 19.581 | -7.795  | 1.00 | 19.66 |
| ATOM | 3264 | CD2 | LEU | 106 | 17.867 | 18.445 | -8.518  | 1.00 | 20.28 |
| ATOM | 3265 | H   | LEU | 106 | 20.026 | 21.246 | -7.491  | 1.00 | 0.00  |
| ATOM | 3266 | N   | GLU | 107 | 19.400 | 22.844 | -11.006 | 1.00 | 21.93 |
| ATOM | 3267 | CA  | GLU | 107 | 19.623 | 24.215 | -11.452 | 1.00 | 24.66 |
| ATOM | 3268 | C   | GLU | 107 | 18.293 | 24.778 | -11.904 | 1.00 | 25.13 |
| ATOM | 3269 | O   | GLU | 107 | 17.572 | 24.129 | -12.664 | 1.00 | 26.66 |
| ATOM | 3270 | CB  | GLU | 107 | 20.631 | 24.252 | -12.614 | 1.00 | 26.28 |
| ATOM | 3271 | CG  | GLU | 107 | 20.927 | 25.657 | -13.160 | 1.00 | 27.29 |
| ATOM | 3272 | CD  | GLU | 107 | 21.953 | 25.661 | -14.289 | 1.00 | 29.17 |
| ATOM | 3273 | OE1 | GLU | 107 | 22.959 | 26.386 | -14.187 | 1.00 | 30.52 |
| ATOM | 3274 | OE2 | GLU | 107 | 21.777 | 24.940 | -15.293 | 1.00 | 31.23 |
| ATOM | 3275 | H   | GLU | 107 | 19.378 | 22.140 | -11.669 | 1.00 | 0.00  |
| ATOM | 3276 | N   | LEU | 108 | 17.948 | 25.966 | -11.422 | 1.00 | 23.99 |
| ATOM | 3277 | CA  | LEU | 108 | 16.689 | 26.587 | -11.803 | 1.00 | 24.64 |
| ATOM | 3278 | C   | LEU | 108 | 16.868 | 27.234 | -13.171 | 1.00 | 29.15 |
| ATOM | 3279 | O   | LEU | 108 | 17.994 | 27.557 | -13.555 | 1.00 | 30.56 |
| ATOM | 3280 | CB  | LEU | 108 | 16.282 | 27.628 | -10.766 | 1.00 | 20.08 |
| ATOM | 3281 | CG  | LEU | 108 | 16.096 | 27.099 | -9.345  | 1.00 | 17.40 |
| ATOM | 3282 | CD1 | LEU | 108 | 15.604 | 28.210 | -8.446  | 1.00 | 17.94 |
| ATOM | 3283 | CD2 | LEU | 108 | 15.110 | 25.953 | -9.327  | 1.00 | 15.86 |
| ATOM | 3284 | H   | LEU | 108 | 18.597 | 26.433 | -10.858 | 1.00 | 0.00  |
| ATOM | 3285 | N   | GLU | 109 | 15.783 | 27.393 | -13.925 | 1.00 | 34.05 |
| ATOM | 3286 | CA  | GLU | 109 | 15.878 | 28.014 | -15.249 | 1.00 | 39.14 |
| ATOM | 3287 | C   | GLU | 109 | 16.218 | 29.495 | -15.112 | 1.00 | 41.66 |
| ATOM | 3288 | O   | GLU | 109 | 16.942 | 30.053 | -15.934 | 1.00 | 42.60 |
| ATOM | 3289 | CB  | GLU | 109 | 14.579 | 27.842 | -16.047 | 1.00 | 41.87 |
| ATOM | 3290 | CG  | GLU | 109 | 14.169 | 26.380 | -16.270 | 1.00 | 47.69 |
| ATOM | 3291 | CD  | GLU | 109 | 14.120 | 25.960 | -17.742 | 1.00 | 50.47 |
| ATOM | 3292 | OE1 | GLU | 109 | 13.324 | 25.050 | -18.074 | 1.00 | 51.05 |
| ATOM | 3293 | OE2 | GLU | 109 | 14.887 | 26.517 | -18.561 | 1.00 | 51.80 |
| ATOM | 3294 | H   | GLU | 109 | 14.908 | 27.060 | -13.609 | 1.00 | 0.00  |
| ATOM | 3295 | N   | GLU | 110 | 15.729 | 30.114 | -14.045 | 1.00 | 44.14 |
| ATOM | 3296 | CA  | GLU | 110 | 15.978 | 31.528 | -13.784 | 1.00 | 47.55 |
| ATOM | 3297 | C   | GLU | 110 | 16.286 | 31.701 | -12.299 | 1.00 | 48.50 |
| ATOM | 3298 | O   | GLU | 110 | 15.821 | 30.916 | -11.467 | 1.00 | 49.30 |
| ATOM | 3299 | CB  | GLU | 110 | 14.744 | 32.357 | -14.154 | 1.00 | 50.55 |
| ATOM | 3300 | CG  | GLU | 110 | 13.481 | 31.919 | -13.414 | 1.00 | 54.94 |
| ATOM | 3301 | CD  | GLU | 110 | 12.254 | 32.729 | -13.785 | 1.00 | 56.79 |
| ATOM | 3302 | OE1 | GLU | 110 | 11.801 | 33.542 | -12.950 | 1.00 | 58.86 |
| ATOM | 3303 | OE2 | GLU | 110 | 11.732 | 32.540 | -14.904 | 1.00 | 57.42 |
| ATOM | 3304 | H   | GLU | 110 | 15.183 | 29.613 | -13.398 | 1.00 | 0.00  |
| ATOM | 3305 | N   | PRO | 111 | 17.128 | 32.687 | -11.952 | 1.00 | 48.50 |
| ATOM | 3306 | CA  | PRO | 111 | 17.479 | 32.931 | -10.550 | 1.00 | 48.59 |
| ATOM | 3307 | C   | PRO | 111 | 16.286 | 33.490 | -9.783  | 1.00 | 49.59 |
| ATOM | 3308 | O   | PRO | 111 | 15.459 | 34.215 | -10.342 | 1.00 | 49.69 |
| ATOM | 3309 | CB  | PRO | 111 | 18.594 | 33.971 | -10.653 | 1.00 | 48.14 |
| ATOM | 3310 | CG  | PRO | 111 | 19.174 | 33.734 | -12.013 | 1.00 | 48.12 |
| ATOM | 3311 | CD  | PRO | 111 | 17.945 | 33.522 | -12.845 | 1.00 | 48.37 |
| ATOM | 3312 | N   | VAL | 112 | 16.201 | 33.153 | -8.505  | 1.00 | 50.84 |
| ATOM | 3313 | CA  | VAL | 112 | 15.110 | 33.622 | -7.668  | 1.00 | 53.38 |
| ATOM | 3314 | C   | VAL | 112 | 15.533 | 34.865 | -6.901  | 1.00 | 56.72 |
| ATOM | 3315 | O   | VAL | 112 | 16.601 | 34.887 | -6.287  | 1.00 | 58.71 |
| ATOM | 3316 | CB  | VAL | 112 | 14.653 | 32.536 | -6.664  | 1.00 | 52.88 |
| ATOM | 3317 | CG1 | VAL | 112 | 14.176 | 31.304 | -7.407  | 1.00 | 53.74 |
| ATOM | 3318 | CG2 | VAL | 112 | 15.776 | 32.173 | -5.708  | 1.00 | 52.31 |
| ATOM | 3319 | H   | VAL | 112 | 16.926 | 32.607 | -8.142  | 1.00 | 0.00  |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3320 | N   | LYS | 113 | 14.722 | 35.917 | -6.970 | 1.00 | 58.96 |
| ATOM | 3321 | CA  | LYS | 113 | 15.022 | 37.152 | -6.248 | 1.00 | 60.41 |
| ATOM | 3322 | C   | LYS | 113 | 14.853 | 36.838 | -4.765 | 1.00 | 60.77 |
| ATOM | 3323 | O   | LYS | 113 | 13.757 | 36.967 | -4.216 | 1.00 | 61.43 |
| ATOM | 3324 | CB  | LYS | 113 | 14.057 | 38.276 | -6.647 | 1.00 | 61.58 |
| ATOM | 3325 | CG  | LYS | 113 | 13.890 | 38.485 | -8.147 | 1.00 | 63.29 |
| ATOM | 3326 | CD  | LYS | 113 | 12.543 | 37.954 | -8.629 | 1.00 | 65.05 |
| ATOM | 3327 | CE  | LYS | 113 | 11.376 | 38.698 | -7.973 | 1.00 | 65.70 |
| ATOM | 3328 | NZ  | LYS | 113 | 10.048 | 38.167 | -8.401 | 1.00 | 66.27 |
| ATOM | 3329 | H   | LYS | 113 | 13.925 | 35.825 | -7.520 | 1.00 | 0.00  |
| ATOM | 3330 | HZ1 | LYS | 113 | 9.962  | 37.166 | -8.136 | 1.00 | 0.00  |
| ATOM | 3331 | HZ2 | LYS | 113 | 9.955  | 38.272 | -9.432 | 1.00 | 0.00  |
| ATOM | 3332 | HZ3 | LYS | 113 | 9.304  | 38.717 | -7.925 | 1.00 | 0.00  |
| ATOM | 3333 | N   | VAL | 114 | 15.925 | 36.360 | -4.147 | 1.00 | 60.71 |
| ATOM | 3334 | CA  | VAL | 114 | 15.908 | 36.001 | -2.738 | 1.00 | 60.67 |
| ATOM | 3335 | C   | VAL | 114 | 15.500 | 37.157 | -1.829 | 1.00 | 60.65 |
| ATOM | 3336 | O   | VAL | 114 | 16.274 | 38.086 | -1.592 | 1.00 | 60.82 |
| ATOM | 3337 | CB  | VAL | 114 | 17.264 | 35.410 | -2.300 | 1.00 | 61.10 |
| ATOM | 3338 | CG1 | VAL | 114 | 17.445 | 34.025 | -2.915 | 1.00 | 61.42 |
| ATOM | 3339 | CG2 | VAL | 114 | 18.408 | 36.323 | -2.726 | 1.00 | 61.09 |
| ATOM | 3340 | H   | VAL | 114 | 16.737 | 36.214 | -4.674 | 1.00 | 0.00  |
| ATOM | 3341 | N   | SER | 115 | 14.267 | 37.102 | -1.340 | 1.00 | 61.08 |
| ATOM | 3342 | CA  | SER | 115 | 13.732 | 38.139 | -0.466 | 1.00 | 61.41 |
| ATOM | 3343 | C   | SER | 115 | 13.957 | 37.844 | 1.021  | 1.00 | 61.79 |
| ATOM | 3344 | O   | SER | 115 | 14.564 | 36.829 | 1.387  | 1.00 | 62.53 |
| ATOM | 3345 | CB  | SER | 115 | 12.238 | 38.347 | -0.752 | 1.00 | 60.84 |
| ATOM | 3346 | OG  | SER | 115 | 11.484 | 37.178 | -0.475 | 1.00 | 60.27 |
| ATOM | 3347 | H   | SER | 115 | 13.706 | 36.338 | -1.597 | 1.00 | 0.00  |
| ATOM | 3348 | HG  | SER | 115 | 11.199 | 37.174 | 0.429  | 1.00 | 0.00  |
| ATOM | 3349 | N   | SER | 116 | 13.436 | 38.720 | 1.876  | 1.00 | 61.44 |
| ATOM | 3350 | CA  | SER | 116 | 13.566 | 38.573 | 3.325  | 1.00 | 61.01 |
| ATOM | 3351 | C   | SER | 116 | 12.974 | 37.259 | 3.839  | 1.00 | 59.89 |
| ATOM | 3352 | O   | SER | 116 | 13.434 | 36.709 | 4.844  | 1.00 | 58.72 |
| ATOM | 3353 | CB  | SER | 116 | 12.889 | 39.756 | 4.028  | 1.00 | 61.11 |
| ATOM | 3354 | OG  | SER | 116 | 11.542 | 39.897 | 3.604  | 1.00 | 61.47 |
| ATOM | 3355 | H   | SER | 116 | 12.965 | 39.513 | 1.546  | 1.00 | 0.00  |
| ATOM | 3356 | HG  | SER | 116 | 11.260 | 40.769 | 3.917  | 1.00 | 0.00  |
| ATOM | 3357 | N   | HIS | 117 | 11.971 | 36.753 | 3.129  | 1.00 | 59.62 |
| ATOM | 3358 | CA  | HIS | 117 | 11.302 | 35.514 | 3.517  | 1.00 | 59.34 |
| ATOM | 3359 | C   | HIS | 117 | 11.737 | 34.297 | 2.695  | 1.00 | 56.48 |
| ATOM | 3360 | O   | HIS | 117 | 11.407 | 33.165 | 3.050  | 1.00 | 56.61 |
| ATOM | 3361 | CB  | HIS | 117 | 9.776  | 35.680 | 3.430  | 1.00 | 63.09 |
| ATOM | 3362 | CG  | HIS | 117 | 9.255  | 36.924 | 4.090  | 1.00 | 66.88 |
| ATOM | 3363 | ND1 | HIS | 117 | 9.417  | 37.184 | 5.436  | 1.00 | 67.62 |
| ATOM | 3364 | CD2 | HIS | 117 | 8.580  | 37.985 | 3.583  | 1.00 | 67.79 |
| ATOM | 3365 | CE1 | HIS | 117 | 8.866  | 38.349 | 5.728  | 1.00 | 68.20 |
| ATOM | 3366 | NE2 | HIS | 117 | 8.352  | 38.855 | 4.622  | 1.00 | 68.20 |
| ATOM | 3367 | H   | HIS | 117 | 11.705 | 37.219 | 2.318  | 1.00 | 0.00  |
| ATOM | 3368 | HD1 | HIS | 117 | 9.878  | 36.624 | 6.106  | 1.00 | 0.00  |
| ATOM | 3369 | HE2 | HIS | 117 | 7.875  | 39.714 | 4.550  | 1.00 | 0.00  |
| ATOM | 3370 | N   | VAL | 118 | 12.467 | 34.527 | 1.604  | 1.00 | 52.48 |
| ATOM | 3371 | CA  | VAL | 118 | 12.937 | 33.444 | 0.739  | 1.00 | 48.37 |
| ATOM | 3372 | C   | VAL | 118 | 14.356 | 33.705 | 0.246  | 1.00 | 46.52 |
| ATOM | 3373 | O   | VAL | 118 | 14.562 | 34.432 | -0.721 | 1.00 | 45.40 |
| ATOM | 3374 | CB  | VAL | 118 | 12.004 | 33.257 | -0.480 | 1.00 | 46.79 |
| ATOM | 3375 | CG1 | VAL | 118 | 12.673 | 32.415 | -1.553 | 1.00 | 46.40 |
| ATOM | 3376 | CG2 | VAL | 118 | 10.720 | 32.593 | -0.041 | 1.00 | 46.79 |
| ATOM | 3377 | H   | VAL | 118 | 12.723 | 35.429 | 1.328  | 1.00 | 0.00  |
| ATOM | 3378 | N   | HIS | 119 | 15.334 | 33.121 | 0.927  | 1.00 | 45.06 |
| ATOM | 3379 | CA  | HIS | 119 | 16.725 | 33.294 | 0.536  | 1.00 | 43.51 |
| ATOM | 3380 | C   | HIS | 119 | 17.584 | 32.079 | 0.860  | 1.00 | 41.34 |
| ATOM | 3381 | O   | HIS | 119 | 17.141 | 31.157 | 1.547  | 1.00 | 41.25 |
| ATOM | 3382 | CB  | HIS | 119 | 17.328 | 34.578 | 1.126  | 1.00 | 44.71 |

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3383 | CG  | HIS | 119 | 17.256 | 34.664 | 2.618  | 1.00 | 45.16 |
| ATOM | 3384 | ND1 | HIS | 119 | 16.287 | 35.392 | 3.273  | 1.00 | 45.96 |
| ATOM | 3385 | CD2 | HIS | 119 | 18.054 | 34.148 | 3.582  | 1.00 | 46.03 |
| ATOM | 3386 | CE1 | HIS | 119 | 16.490 | 35.324 | 4.576  | 1.00 | 47.16 |
| ATOM | 3387 | NE2 | HIS | 119 | 17.558 | 34.575 | 4.790  | 1.00 | 47.71 |
| ATOM | 3388 | H   | HIS | 119 | 15.120 | 32.488 | 1.647  | 1.00 | 0.00  |
| ATOM | 3389 | HD1 | HIS | 119 | 15.585 | 35.902 | 2.803  | 1.00 | 0.00  |
| ATOM | 3390 | HE2 | HIS | 119 | 17.950 | 34.357 | 5.664  | 1.00 | 0.00  |
| ATOM | 3391 | N   | THR | 120 | 18.819 | 32.106 | 0.372  | 1.00 | 38.34 |
| ATOM | 3392 | CA  | THR | 120 | 19.766 | 31.013 | 0.541  | 1.00 | 34.55 |
| ATOM | 3393 | C   | THR | 120 | 20.300 | 30.749 | 1.943  | 1.00 | 32.22 |
| ATOM | 3394 | O   | THR | 120 | 20.341 | 31.640 | 2.790  | 1.00 | 33.28 |
| ATOM | 3395 | CB  | THR | 120 | 20.957 | 31.205 | -0.399 | 1.00 | 33.14 |
| ATOM | 3396 | OG1 | THR | 120 | 21.644 | 32.412 | -0.057 | 1.00 | 31.99 |
| ATOM | 3397 | CG2 | THR | 120 | 20.468 | 31.317 | -1.823 | 1.00 | 31.97 |
| ATOM | 3398 | H   | THR | 120 | 19.128 | 32.885 | -0.127 | 1.00 | 0.00  |
| ATOM | 3399 | HG1 | THR | 120 | 21.164 | 33.191 | -0.368 | 1.00 | 0.00  |
| ATOM | 3400 | N   | VAL | 121 | 20.679 | 29.497 | 2.181  | 1.00 | 29.15 |
| ATOM | 3401 | CA  | VAL | 121 | 21.254 | 29.085 | 3.452  | 1.00 | 27.82 |
| ATOM | 3402 | C   | VAL | 121 | 22.755 | 29.234 | 3.250  | 1.00 | 28.37 |
| ATOM | 3403 | O   | VAL | 121 | 23.207 | 29.538 | 2.145  | 1.00 | 28.69 |
| ATOM | 3404 | CB  | VAL | 121 | 20.902 | 27.613 | 3.795  | 1.00 | 26.96 |
| ATOM | 3405 | CG1 | VAL | 121 | 21.481 | 26.673 | 2.764  | 1.00 | 27.49 |
| ATOM | 3406 | CG2 | VAL | 121 | 21.379 | 27.247 | 5.196  | 1.00 | 24.97 |
| ATOM | 3407 | H   | VAL | 121 | 20.573 | 28.879 | 1.433  | 1.00 | 0.00  |
| ATOM | 3408 | N   | THR | 122 | 23.532 | 29.039 | 4.303  | 1.00 | 29.72 |
| ATOM | 3409 | CA  | THR | 122 | 24.969 | 29.171 | 4.183  | 1.00 | 31.59 |
| ATOM | 3410 | C   | THR | 122 | 25.618 | 27.802 | 4.349  | 1.00 | 32.19 |
| ATOM | 3411 | O   | THR | 122 | 25.270 | 27.053 | 5.269  | 1.00 | 32.90 |
| ATOM | 3412 | CB  | THR | 122 | 25.516 | 30.143 | 5.246  | 1.00 | 33.10 |
| ATOM | 3413 | OG1 | THR | 122 | 24.646 | 31.280 | 5.354  | 1.00 | 34.19 |
| ATOM | 3414 | CG2 | THR | 122 | 26.904 | 30.624 | 4.855  | 1.00 | 33.93 |
| ATOM | 3415 | H   | THR | 122 | 23.207 | 28.833 | 5.203  | 1.00 | 0.00  |
| ATOM | 3416 | HG1 | THR | 122 | 23.766 | 31.001 | 5.612  | 1.00 | 0.00  |
| ATOM | 3417 | N   | LEU | 123 | 26.515 | 27.452 | 3.430  | 1.00 | 31.53 |
| ATOM | 3418 | CA  | LEU | 123 | 27.209 | 26.167 | 3.496  | 1.00 | 31.02 |
| ATOM | 3419 | C   | LEU | 123 | 28.322 | 26.220 | 4.548  | 1.00 | 31.62 |
| ATOM | 3420 | O   | LEU | 123 | 29.049 | 27.204 | 4.661  | 1.00 | 32.50 |
| ATOM | 3421 | CB  | LEU | 123 | 27.773 | 25.771 | 2.121  | 1.00 | 29.42 |
| ATOM | 3422 | CG  | LEU | 123 | 26.790 | 25.351 | 1.019  | 1.00 | 26.99 |
| ATOM | 3423 | CD1 | LEU | 123 | 27.539 | 25.158 | -0.291 | 1.00 | 25.06 |
| ATOM | 3424 | CD2 | LEU | 123 | 26.053 | 24.076 | 1.416  | 1.00 | 24.67 |
| ATOM | 3425 | H   | LEU | 123 | 26.732 | 28.064 | 2.703  | 1.00 | 0.00  |
| ATOM | 3426 | N   | PRO | 124 | 28.448 | 25.164 | 5.354  | 1.00 | 32.64 |
| ATOM | 3427 | CA  | PRO | 124 | 29.466 | 25.094 | 6.400  | 1.00 | 34.01 |
| ATOM | 3428 | C   | PRO | 124 | 30.865 | 25.195 | 5.836  | 1.00 | 35.14 |
| ATOM | 3429 | O   | PRO | 124 | 31.122 | 24.755 | 4.725  | 1.00 | 34.65 |
| ATOM | 3430 | CB  | PRO | 124 | 29.232 | 23.711 | 6.998  | 1.00 | 33.70 |
| ATOM | 3431 | CG  | PRO | 124 | 28.733 | 22.933 | 5.818  | 1.00 | 32.32 |
| ATOM | 3432 | CD  | PRO | 124 | 27.740 | 23.882 | 5.238  | 1.00 | 32.80 |
| ATOM | 3433 | N   | PRO | 125 | 31.782 | 25.814 | 6.585  | 1.00 | 37.49 |
| ATOM | 3434 | CA  | PRO | 125 | 33.155 | 25.934 | 6.103  | 1.00 | 39.11 |
| ATOM | 3435 | C   | PRO | 125 | 33.768 | 24.534 | 6.072  | 1.00 | 40.69 |
| ATOM | 3436 | O   | PRO | 125 | 33.358 | 23.655 | 6.828  | 1.00 | 39.70 |
| ATOM | 3437 | CB  | PRO | 125 | 33.806 | 26.813 | 7.168  | 1.00 | 38.93 |
| ATOM | 3438 | CG  | PRO | 125 | 33.057 | 26.451 | 8.404  | 1.00 | 38.22 |
| ATOM | 3439 | CD  | PRO | 125 | 31.637 | 26.440 | 7.907  | 1.00 | 38.30 |
| ATOM | 3440 | N   | ALA | 126 | 34.750 | 24.340 | 5.202  | 1.00 | 43.31 |
| ATOM | 3441 | CA  | ALA | 126 | 35.410 | 23.048 | 5.054  | 1.00 | 46.91 |
| ATOM | 3442 | C   | ALA | 126 | 35.841 | 22.416 | 6.378  | 1.00 | 49.80 |
| ATOM | 3443 | O   | ALA | 126 | 35.583 | 21.238 | 6.633  | 1.00 | 49.92 |
| ATOM | 3444 | CB  | ALA | 126 | 36.606 | 23.185 | 4.121  | 1.00 | 47.29 |
| ATOM | 3445 | H   | ALA | 126 | 35.003 | 25.084 | 4.619  | 1.00 | 0.00  |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3446 | N   | SER | 127 | 36.471 | 23.220 | 7.228  | 1.00 | 52.56 |
| ATOM | 3447 | CA  | SER | 127 | 36.965 | 22.758 | 8.521  | 1.00 | 54.03 |
| ATOM | 3448 | C   | SER | 127 | 35.882 | 22.529 | 9.567  | 1.00 | 53.77 |
| ATOM | 3449 | O   | SER | 127 | 36.141 | 21.913 | 10.604 | 1.00 | 54.33 |
| ATOM | 3450 | CB  | SER | 127 | 38.012 | 23.748 | 9.062  | 1.00 | 55.86 |
| ATOM | 3451 | OG  | SER | 127 | 37.547 | 25.096 | 9.042  | 1.00 | 55.97 |
| ATOM | 3452 | H   | SER | 127 | 36.613 | 24.162 | 7.017  | 1.00 | 0.00  |
| ATOM | 3453 | HG  | SER | 127 | 36.899 | 25.219 | 9.754  | 1.00 | 0.00  |
| ATOM | 3454 | N   | GLU | 128 | 34.667 | 22.982 | 9.283  | 1.00 | 53.27 |
| ATOM | 3455 | CA  | GLU | 128 | 33.584 | 22.845 | 10.242 | 1.00 | 52.57 |
| ATOM | 3456 | C   | GLU | 128 | 33.379 | 21.431 | 10.738 | 1.00 | 51.46 |
| ATOM | 3457 | O   | GLU | 128 | 33.433 | 20.464 | 9.974  | 1.00 | 51.06 |
| ATOM | 3458 | CB  | GLU | 128 | 32.280 | 23.412 | 9.694  | 1.00 | 53.36 |
| ATOM | 3459 | CG  | GLU | 128 | 31.271 | 23.725 | 10.784 | 1.00 | 54.12 |
| ATOM | 3460 | CD  | GLU | 128 | 31.896 | 24.467 | 11.957 | 1.00 | 53.62 |
| ATOM | 3461 | OE1 | GLU | 128 | 32.412 | 25.586 | 11.755 | 1.00 | 53.92 |
| ATOM | 3462 | OE2 | GLU | 128 | 31.892 | 23.916 | 13.076 | 1.00 | 54.19 |
| ATOM | 3463 | H   | GLU | 128 | 34.461 | 23.358 | 8.410  | 1.00 | 0.00  |
| ATOM | 3464 | N   | THR | 129 | 33.158 | 21.330 | 12.039 | 1.00 | 50.59 |
| ATOM | 3465 | CA  | THR | 129 | 32.957 | 20.056 | 12.697 | 1.00 | 50.23 |
| ATOM | 3466 | C   | THR | 129 | 31.897 | 20.296 | 13.752 | 1.00 | 48.52 |
| ATOM | 3467 | O   | THR | 129 | 32.040 | 21.174 | 14.607 | 1.00 | 49.08 |
| ATOM | 3468 | CB  | THR | 129 | 34.258 | 19.566 | 13.375 | 1.00 | 51.98 |
| ATOM | 3469 | OG1 | THR | 129 | 35.310 | 19.488 | 12.403 | 1.00 | 52.92 |
| ATOM | 3470 | CG2 | THR | 129 | 34.047 | 18.191 | 14.005 | 1.00 | 53.49 |
| ATOM | 3471 | H   | THR | 129 | 33.075 | 22.147 | 12.589 | 1.00 | 0.00  |
| ATOM | 3472 | HG1 | THR | 129 | 35.517 | 20.322 | 11.951 | 1.00 | 0.00  |
| ATOM | 3473 | N   | PHE | 130 | 30.828 | 19.517 | 13.687 | 1.00 | 45.94 |
| ATOM | 3474 | CA  | PHE | 130 | 29.729 | 19.646 | 14.626 | 1.00 | 42.95 |
| ATOM | 3475 | C   | PHE | 130 | 29.930 | 18.670 | 15.774 | 1.00 | 41.42 |
| ATOM | 3476 | O   | PHE | 130 | 29.925 | 17.448 | 15.588 | 1.00 | 41.86 |
| ATOM | 3477 | CB  | PHE | 130 | 28.408 | 19.423 | 13.889 | 1.00 | 41.39 |
| ATOM | 3478 | CG  | PHE | 130 | 28.266 | 20.285 | 12.672 | 1.00 | 39.34 |
| ATOM | 3479 | CD1 | PHE | 130 | 29.033 | 20.029 | 11.535 | 1.00 | 38.47 |
| ATOM | 3480 | CD2 | PHE | 130 | 27.435 | 21.400 | 12.681 | 1.00 | 38.73 |
| ATOM | 3481 | CE1 | PHE | 130 | 28.977 | 20.874 | 10.429 | 1.00 | 38.13 |
| ATOM | 3482 | CE2 | PHE | 130 | 27.375 | 22.247 | 11.576 | 1.00 | 38.62 |
| ATOM | 3483 | CZ  | PHE | 130 | 28.149 | 21.985 | 10.452 | 1.00 | 37.77 |
| ATOM | 3484 | H   | PHE | 130 | 30.776 | 18.819 | 13.005 | 1.00 | 0.00  |
| ATOM | 3485 | N   | PRO | 131 | 30.188 | 19.205 | 16.974 | 1.00 | 39.65 |
| ATOM | 3486 | CA  | PRO | 131 | 30.415 | 18.422 | 18.191 | 1.00 | 39.34 |
| ATOM | 3487 | C   | PRO | 131 | 29.215 | 17.585 | 18.606 | 1.00 | 37.64 |
| ATOM | 3488 | O   | PRO | 131 | 28.074 | 18.028 | 18.509 | 1.00 | 36.77 |
| ATOM | 3489 | CB  | PRO | 131 | 30.736 | 19.497 | 19.230 | 1.00 | 40.21 |
| ATOM | 3490 | CG  | PRO | 131 | 29.932 | 20.666 | 18.755 | 1.00 | 40.85 |
| ATOM | 3491 | CD  | PRO | 131 | 30.192 | 20.647 | 17.272 | 1.00 | 39.74 |
| ATOM | 3492 | N   | PRO | 132 | 29.466 | 16.377 | 19.121 | 1.00 | 37.42 |
| ATOM | 3493 | CA  | PRO | 132 | 28.375 | 15.504 | 19.550 | 1.00 | 37.72 |
| ATOM | 3494 | C   | PRO | 132 | 27.533 | 16.249 | 20.565 | 1.00 | 38.37 |
| ATOM | 3495 | O   | PRO | 132 | 28.054 | 17.001 | 21.398 | 1.00 | 38.89 |
| ATOM | 3496 | CB  | PRO | 132 | 29.112 | 14.327 | 20.184 | 1.00 | 37.73 |
| ATOM | 3497 | CG  | PRO | 132 | 30.364 | 14.965 | 20.711 | 1.00 | 37.59 |
| ATOM | 3498 | CD  | PRO | 132 | 30.766 | 15.844 | 19.563 | 1.00 | 37.40 |
| ATOM | 3499 | N   | GLY | 133 | 26.225 | 16.077 | 20.479 | 1.00 | 39.47 |
| ATOM | 3500 | CA  | GLY | 133 | 25.351 | 16.763 | 21.399 | 1.00 | 41.19 |
| ATOM | 3501 | C   | GLY | 133 | 24.882 | 18.096 | 20.850 | 1.00 | 42.36 |
| ATOM | 3502 | O   | GLY | 133 | 23.771 | 18.519 | 21.172 | 1.00 | 44.14 |
| ATOM | 3503 | H   | GLY | 133 | 25.850 | 15.490 | 19.787 | 1.00 | 0.00  |
| ATOM | 3504 | N   | MET | 134 | 25.701 | 18.756 | 20.029 | 1.00 | 41.67 |
| ATOM | 3505 | CA  | MET | 134 | 25.311 | 20.043 | 19.455 | 1.00 | 41.10 |
| ATOM | 3506 | C   | MET | 134 | 23.939 | 19.873 | 18.821 | 1.00 | 41.05 |
| ATOM | 3507 | O   | MET | 134 | 23.740 | 19.000 | 17.968 | 1.00 | 41.93 |
| ATOM | 3508 | CB  | MET | 134 | 26.309 | 20.505 | 18.395 | 1.00 | 41.54 |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3509 | CG  | MET | 134 | 25.883 | 21.760 | 17.658 | 1.00 | 43.25 |
| ATOM | 3510 | SD  | MET | 134 | 27.021 | 22.197 | 16.336 | 1.00 | 47.72 |
| ATOM | 3511 | CE  | MET | 134 | 27.509 | 23.857 | 16.830 | 1.00 | 47.53 |
| ATOM | 3512 | H   | MET | 134 | 26.553 | 18.382 | 19.728 | 1.00 | 0.00  |
| ATOM | 3513 | N   | PRO | 135 | 22.950 | 20.634 | 19.302 | 1.00 | 39.34 |
| ATOM | 3514 | CA  | PRO | 135 | 21.611 | 20.507 | 18.731 | 1.00 | 37.12 |
| ATOM | 3515 | C   | PRO | 135 | 21.502 | 21.224 | 17.398 | 1.00 | 34.98 |
| ATOM | 3516 | O   | PRO | 135 | 21.989 | 22.345 | 17.231 | 1.00 | 34.48 |
| ATOM | 3517 | CB  | PRO | 135 | 20.730 | 21.143 | 19.799 | 1.00 | 36.81 |
| ATOM | 3518 | CG  | PRO | 135 | 21.597 | 22.242 | 20.312 | 1.00 | 39.01 |
| ATOM | 3519 | CD  | PRO | 135 | 22.961 | 21.584 | 20.429 | 1.00 | 39.13 |
| ATOM | 3520 | N   | CYS | 136 | 20.911 | 20.537 | 16.439 | 1.00 | 33.50 |
| ATOM | 3521 | CA  | CYS | 136 | 20.695 | 21.083 | 15.117 | 1.00 | 32.45 |
| ATOM | 3522 | C   | CYS | 136 | 19.210 | 20.890 | 14.843 | 1.00 | 33.73 |
| ATOM | 3523 | O   | CYS | 136 | 18.495 | 20.337 | 15.684 | 1.00 | 34.39 |
| ATOM | 3524 | CB  | CYS | 136 | 21.544 | 20.335 | 14.098 | 1.00 | 30.37 |
| ATOM | 3525 | SG  | CYS | 136 | 23.334 | 20.503 | 14.358 | 1.00 | 26.22 |
| ATOM | 3526 | H   | CYS | 136 | 20.625 | 19.625 | 16.608 | 1.00 | 0.00  |
| ATOM | 3527 | N   | TRP | 137 | 18.738 | 21.344 | 13.686 | 1.00 | 33.94 |
| ATOM | 3528 | CA  | TRP | 137 | 17.324 | 21.224 | 13.342 | 1.00 | 33.40 |
| ATOM | 3529 | C   | TRP | 137 | 17.145 | 20.648 | 11.952 | 1.00 | 33.84 |
| ATOM | 3530 | O   | TRP | 137 | 17.884 | 21.003 | 11.037 | 1.00 | 35.74 |
| ATOM | 3531 | CB  | TRP | 137 | 16.656 | 22.600 | 13.352 | 1.00 | 33.55 |
| ATOM | 3532 | CG  | TRP | 137 | 16.834 | 23.404 | 14.600 | 1.00 | 32.89 |
| ATOM | 3533 | CD1 | TRP | 137 | 17.993 | 23.951 | 15.072 | 1.00 | 32.81 |
| ATOM | 3534 | CD2 | TRP | 137 | 15.809 | 23.789 | 15.512 | 1.00 | 33.22 |
| ATOM | 3535 | NE1 | TRP | 137 | 17.750 | 24.657 | 16.221 | 1.00 | 32.46 |
| ATOM | 3536 | CE2 | TRP | 137 | 16.416 | 24.575 | 16.515 | 1.00 | 32.62 |
| ATOM | 3537 | CE3 | TRP | 137 | 14.431 | 23.547 | 15.579 | 1.00 | 34.85 |
| ATOM | 3538 | CZ2 | TRP | 137 | 15.696 | 25.120 | 17.572 | 1.00 | 34.22 |
| ATOM | 3539 | CZ3 | TRP | 137 | 13.709 | 24.090 | 16.635 | 1.00 | 35.32 |
| ATOM | 3540 | CH2 | TRP | 137 | 14.345 | 24.869 | 17.617 | 1.00 | 35.81 |
| ATOM | 3541 | H   | TRP | 137 | 19.351 | 21.782 | 13.054 | 1.00 | 0.00  |
| ATOM | 3542 | HE1 | TRP | 137 | 18.442 | 25.193 | 16.667 | 1.00 | 0.00  |
| ATOM | 3543 | N   | VAL | 138 | 16.159 | 19.773 | 11.796 | 1.00 | 34.21 |
| ATOM | 3544 | CA  | VAL | 138 | 15.846 | 19.179 | 10.495 | 1.00 | 34.78 |
| ATOM | 3545 | C   | VAL | 138 | 14.489 | 19.779 | 10.144 | 1.00 | 35.19 |
| ATOM | 3546 | O   | VAL | 138 | 13.687 | 20.056 | 11.045 | 1.00 | 36.78 |
| ATOM | 3547 | CB  | VAL | 138 | 15.679 | 17.649 | 10.566 | 1.00 | 35.29 |
| ATOM | 3548 | CG1 | VAL | 138 | 15.790 | 17.049 | 9.182  | 1.00 | 35.55 |
| ATOM | 3549 | CG2 | VAL | 138 | 16.703 | 17.040 | 11.485 | 1.00 | 37.18 |
| ATOM | 3550 | H   | VAL | 138 | 15.622 | 19.557 | 12.586 | 1.00 | 0.00  |
| ATOM | 3551 | N   | THR | 139 | 14.216 | 19.972 | 8.859  | 1.00 | 33.49 |
| ATOM | 3552 | CA  | THR | 139 | 12.941 | 20.562 | 8.461  | 1.00 | 32.04 |
| ATOM | 3553 | C   | THR | 139 | 12.356 | 19.855 | 7.242  | 1.00 | 31.06 |
| ATOM | 3554 | O   | THR | 139 | 13.100 | 19.430 | 6.354  | 1.00 | 31.55 |
| ATOM | 3555 | CB  | THR | 139 | 13.110 | 22.066 | 8.140  | 1.00 | 32.20 |
| ATOM | 3556 | OG1 | THR | 139 | 14.107 | 22.641 | 8.995  | 1.00 | 32.70 |
| ATOM | 3557 | CG2 | THR | 139 | 11.811 | 22.795 | 8.374  | 1.00 | 34.44 |
| ATOM | 3558 | H   | THR | 139 | 14.870 | 19.715 | 8.173  | 1.00 | 0.00  |
| ATOM | 3559 | HG1 | THR | 139 | 14.890 | 22.078 | 8.934  | 1.00 | 0.00  |
| ATOM | 3560 | N   | GLY | 140 | 11.030 | 19.740 | 7.194  | 1.00 | 29.01 |
| ATOM | 3561 | CA  | GLY | 140 | 10.390 | 19.083 | 6.064  | 1.00 | 26.53 |
| ATOM | 3562 | C   | GLY | 140 | 8.877  | 19.000 | 6.153  | 1.00 | 24.44 |
| ATOM | 3563 | O   | GLY | 140 | 8.268  | 19.568 | 7.051  | 1.00 | 26.54 |
| ATOM | 3564 | H   | GLY | 140 | 10.475 | 20.083 | 7.932  | 1.00 | 0.00  |
| ATOM | 3565 | N   | TRP | 141 | 8.272  | 18.301 | 5.200  | 1.00 | 21.59 |
| ATOM | 3566 | CA  | TRP | 141 | 6.822  | 18.122 | 5.138  | 1.00 | 18.01 |
| ATOM | 3567 | C   | TRP | 141 | 6.544  | 16.627 | 5.042  | 1.00 | 17.35 |
| ATOM | 3568 | O   | TRP | 141 | 5.624  | 16.201 | 4.334  | 1.00 | 17.29 |
| ATOM | 3569 | CB  | TRP | 141 | 6.256  | 18.778 | 3.875  | 1.00 | 15.10 |
| ATOM | 3570 | CG  | TRP | 141 | 6.260  | 20.267 | 3.834  | 1.00 | 13.29 |
| ATOM | 3571 | CD1 | TRP | 141 | 5.328  | 21.097 | 4.379  | 1.00 | 13.90 |

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|------|------|------|-----|-----|-------|--------|--------|------|-------|
| ATOM | 3572 | CD2  | TRP | 141 | 7.169 | 21.107 | 3.106  | 1.00 | 12.66 |
| ATOM | 3573 | NE1  | TRP | 141 | 5.589 | 22.399 | 4.023  | 1.00 | 13.85 |
| ATOM | 3574 | CE2  | TRP | 141 | 6.712 | 22.434 | 3.244  | 1.00 | 11.73 |
| ATOM | 3575 | CE3  | TRP | 141 | 8.318 | 20.866 | 2.345  | 1.00 | 13.90 |
| ATOM | 3576 | CZ2  | TRP | 141 | 7.360 | 23.514 | 2.650  | 1.00 | 11.79 |
| ATOM | 3577 | CZ3  | TRP | 141 | 8.968 | 21.944 | 1.751  | 1.00 | 13.55 |
| ATOM | 3578 | CH2  | TRP | 141 | 8.486 | 23.250 | 1.909  | 1.00 | 13.61 |
| ATOM | 3579 | H    | TRP | 141 | 8.847 | 17.848 | 4.553  | 1.00 | 0.00  |
| ATOM | 3580 | HE1  | TRP | 141 | 5.064 | 23.185 | 4.278  | 1.00 | 0.00  |
| ATOM | 3581 | N    | GLY | 142 | 7.375 | 15.828 | 5.699  | 1.00 | 16.09 |
| ATOM | 3582 | CA   | GLY | 142 | 7.202 | 14.392 | 5.637  | 1.00 | 16.14 |
| ATOM | 3583 | C    | GLY | 142 | 6.307 | 13.802 | 6.702  | 1.00 | 17.47 |
| ATOM | 3584 | O    | GLY | 142 | 5.665 | 14.520 | 7.469  | 1.00 | 18.32 |
| ATOM | 3585 | H    | GLY | 142 | 8.113 | 16.160 | 6.259  | 1.00 | 0.00  |
| ATOM | 3586 | N    | ASP | 143 | 6.272 | 12.475 | 6.735  | 1.00 | 18.35 |
| ATOM | 3587 | CA   | ASP | 143 | 5.479 | 11.720 | 7.690  | 1.00 | 19.12 |
| ATOM | 3588 | C    | ASP | 143 | 5.818 | 12.116 | 9.115  | 1.00 | 20.80 |
| ATOM | 3589 | O    | ASP | 143 | 6.978 | 12.380 | 9.446  | 1.00 | 20.56 |
| ATOM | 3590 | CB   | ASP | 143 | 5.728 | 10.217 | 7.527  | 1.00 | 19.03 |
| ATOM | 3591 | CG   | ASP | 143 | 5.233 | 9.673  | 6.201  | 1.00 | 18.70 |
| ATOM | 3592 | OD1  | ASP | 143 | 4.551 | 10.410 | 5.448  | 1.00 | 19.38 |
| ATOM | 3593 | OD2  | ASP | 143 | 5.529 | 8.493  | 5.920  | 1.00 | 18.75 |
| ATOM | 3594 | H    | ASP | 143 | 6.807 | 11.996 | 6.066  | 1.00 | 0.00  |
| ATOM | 3595 | N    | VAL | 144 | 4.800 | 12.108 | 9.964  | 1.00 | 22.30 |
| ATOM | 3596 | CA   | VAL | 144 | 4.951 | 12.473 | 11.358 | 1.00 | 23.24 |
| ATOM | 3597 | C    | VAL | 144 | 5.292 | 11.281 | 12.236 | 1.00 | 25.57 |
| ATOM | 3598 | O    | VAL | 144 | 5.557 | 11.442 | 13.426 | 1.00 | 26.10 |
| ATOM | 3599 | CB   | VAL | 144 | 3.688 | 13.143 | 11.871 | 1.00 | 21.79 |
| ATOM | 3600 | CG1  | VAL | 144 | 3.441 | 14.423 | 11.094 | 1.00 | 21.10 |
| ATOM | 3601 | CG2  | VAL | 144 | 2.509 | 12.201 | 11.737 | 1.00 | 20.47 |
| ATOM | 3602 | H    | VAL | 144 | 3.953 | 11.795 | 9.605  | 1.00 | 0.00  |
| ATOM | 3603 | N    | ASP | 145 | 5.271 | 10.095 | 11.642 | 1.00 | 29.19 |
| ATOM | 3604 | CA   | ASP | 145 | 5.590 | 8.841  | 12.325 | 1.00 | 34.16 |
| ATOM | 3605 | C    | ASP | 145 | 5.562 | 7.790  | 11.220 | 1.00 | 36.85 |
| ATOM | 3606 | O    | ASP | 145 | 5.097 | 8.076  | 10.114 | 1.00 | 38.94 |
| ATOM | 3607 | CB   | ASP | 145 | 4.536 | 8.513  | 13.391 | 1.00 | 36.58 |
| ATOM | 3608 | CG   | ASP | 145 | 5.024 | 7.493  | 14.421 | 1.00 | 39.98 |
| ATOM | 3609 | OD1  | ASP | 145 | 5.675 | 6.493  | 14.049 | 1.00 | 42.07 |
| ATOM | 3610 | OD2  | ASP | 145 | 4.760 | 7.691  | 15.624 | 1.00 | 41.75 |
| ATOM | 3611 | H    | ASP | 145 | 5.012 | 10.034 | 10.696 | 1.00 | 0.00  |
| ATOM | 3612 | N    | ASN | 146 | 6.102 | 6.604  | 11.484 | 1.00 | 37.99 |
| ATOM | 3613 | CA   | ASN | 146 | 6.112 | 5.531  | 10.493 | 1.00 | 40.65 |
| ATOM | 3614 | C    | ASN | 146 | 4.690 | 5.290  | 9.989  | 1.00 | 41.93 |
| ATOM | 3615 | O    | ASN | 146 | 3.798 | 4.951  | 10.769 | 1.00 | 42.73 |
| ATOM | 3616 | CB   | ASN | 146 | 6.684 | 4.241  | 11.099 | 1.00 | 42.59 |
| ATOM | 3617 | CG   | ASN | 146 | 8.114 | 4.405  | 11.593 | 1.00 | 44.98 |
| ATOM | 3618 | OD1  | ASN | 146 | 9.078 | 4.147  | 10.866 | 1.00 | 45.48 |
| ATOM | 3619 | ND2  | ASN | 146 | 8.256 | 4.858  | 12.832 | 1.00 | 46.50 |
| ATOM | 3620 | H    | ASN | 146 | 6.501 | 6.482  | 12.364 | 1.00 | 0.00  |
| ATOM | 3621 | HD21 | ASN | 146 | 7.433 | 5.081  | 13.338 | 1.00 | 0.00  |
| ATOM | 3622 | HD22 | ASN | 146 | 9.151 | 4.976  | 13.213 | 1.00 | 0.00  |
| ATOM | 3623 | N    | ASP | 147 | 4.483 | 5.516  | 8.695  | 1.00 | 42.89 |
| ATOM | 3624 | CA   | ASP | 147 | 3.182 | 5.348  | 8.051  | 1.00 | 43.77 |
| ATOM | 3625 | C    | ASP | 147 | 2.153 | 6.353  | 8.526  | 1.00 | 43.61 |
| ATOM | 3626 | O    | ASP | 147 | 0.952 | 6.112  | 8.441  | 1.00 | 45.41 |
| ATOM | 3627 | CB   | ASP | 147 | 2.635 | 3.929  | 8.236  | 1.00 | 46.19 |
| ATOM | 3628 | CG   | ASP | 147 | 3.266 | 2.935  | 7.290  | 1.00 | 49.04 |
| ATOM | 3629 | OD1  | ASP | 147 | 3.502 | 3.289  | 6.111  | 1.00 | 49.80 |
| ATOM | 3630 | OD2  | ASP | 147 | 3.528 | 1.793  | 7.727  | 1.00 | 50.69 |
| ATOM | 3631 | H    | ASP | 147 | 5.215 | 5.831  | 8.129  | 1.00 | 0.00  |
| ATOM | 3632 | N    | GLU | 149 | 2.619 | 7.489  | 9.017  | 1.00 | 42.94 |
| ATOM | 3633 | CA   | GLU | 149 | 1.723 | 8.527  | 9.485  | 1.00 | 43.32 |
| ATOM | 3634 | C    | GLU | 149 | 1.942 | 9.752  | 8.633  | 1.00 | 42.86 |

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|------|------|------|-----|------|--------|--------|--------|------|-------|
| ATOM | 3635 | O    | GLU | 149  | 2.821  | 10.557 | 8.924  | 1.00 | 43.45 |
| ATOM | 3636 | CB   | GLU | 149  | 2.005  | 8.859  | 10.942 | 1.00 | 45.78 |
| ATOM | 3637 | CG   | GLU | 149  | 1.350  | 7.925  | 11.931 | 1.00 | 50.19 |
| ATOM | 3638 | CD   | GLU | 149  | 0.491  | 8.671  | 12.933 | 1.00 | 52.83 |
| ATOM | 3639 | OE1  | GLU | 149  | -0.392 | 9.447  | 12.497 | 1.00 | 55.40 |
| ATOM | 3640 | OE2  | GLU | 149  | 0.695  | 8.488  | 14.153 | 1.00 | 54.00 |
| ATOM | 3641 | H    | GLU | 149  | 3.580  | 7.654  | 9.060  | 1.00 | 0.00  |
| ATOM | 3642 | N    | ARG | 150  | 1.172  | 9.876  | 7.559  | 1.00 | 41.94 |
| ATOM | 3643 | CA   | ARG | 150  | 1.294  | 11.020 | 6.663  | 1.00 | 41.29 |
| ATOM | 3644 | C    | ARG | 150  | 1.051  | 12.332 | 7.400  | 1.00 | 37.71 |
| ATOM | 3645 | O    | ARG | 150  | 0.392  | 12.358 | 8.443  | 1.00 | 37.36 |
| ATOM | 3646 | CB   | ARG | 150  | 0.284  | 10.927 | 5.514  | 1.00 | 45.83 |
| ATOM | 3647 | CG   | ARG | 150  | 0.716  | 10.127 | 4.294  | 1.00 | 51.41 |
| ATOM | 3648 | CD   | ARG | 150  | -0.297 | 10.305 | 3.142  | 1.00 | 56.94 |
| ATOM | 3649 | NE   | ARG | 150  | -0.309 | 11.664 | 2.578  | 1.00 | 61.35 |
| ATOM | 3650 | CZ   | ARG | 150  | -1.307 | 12.545 | 2.711  | 1.00 | 63.02 |
| ATOM | 3651 | NH1  | ARG | 150  | -2.406 | 12.229 | 3.396  | 1.00 | 63.70 |
| ATOM | 3652 | NH2  | ARG | 150  | -1.203 | 13.749 | 2.151  | 1.00 | 62.91 |
| ATOM | 3653 | H    | ARG | 150  | 0.511  | 9.174  | 7.402  | 1.00 | 0.00  |
| ATOM | 3654 | HE   | ARG | 150  | 0.500  | 11.913 | 2.079  | 1.00 | 0.00  |
| ATOM | 3655 | HH11 | ARG | 150  | -2.497 | 11.328 | 3.827  | 1.00 | 0.00  |
| ATOM | 3656 | HH12 | ARG | 150  | -3.179 | 12.853 | 3.521  | 1.00 | 0.00  |
| ATOM | 3657 | HH21 | ARG | 150  | -0.397 | 14.023 | 1.608  | 1.00 | 0.00  |
| ATOM | 3658 | HH22 | ARG | 150  | -1.919 | 14.441 | 2.229  | 1.00 | 0.00  |
| ATOM | 3659 | N    | LEU | 151  | 1.606  | 13.412 | 6.862  | 1.00 | 33.58 |
| ATOM | 3660 | CA   | LEU | 151  | 1.415  | 14.738 | 7.434  | 1.00 | 30.33 |
| ATOM | 3661 | C    | LEU | 151  | 0.016  | 15.146 | 6.998  | 1.00 | 29.75 |
| ATOM | 3662 | O    | LEU | 151  | -0.240 | 15.359 | 5.810  | 1.00 | 32.33 |
| ATOM | 3663 | CB   | LEU | 151  | 2.438  | 15.718 | 6.857  | 1.00 | 29.57 |
| ATOM | 3664 | CG   | LEU | 151  | 2.288  | 17.196 | 7.227  | 1.00 | 28.37 |
| ATOM | 3665 | CD1  | LEU | 151  | 2.698  | 17.417 | 8.671  | 1.00 | 27.54 |
| ATOM | 3666 | CD2  | LEU | 151  | 3.136  | 18.049 | 6.295  | 1.00 | 27.57 |
| ATOM | 3667 | H    | LEU | 151  | 2.183  | 13.304 | 6.079  | 1.00 | 0.00  |
| ATOM | 3668 | N    | PRO | 152  | -0.920 | 15.231 | 7.942  | 1.00 | 27.48 |
| ATOM | 3669 | CA   | PRO | 152  | -2.289 | 15.612 | 7.600  | 1.00 | 25.97 |
| ATOM | 3670 | C    | PRO | 152  | -2.425 | 17.049 | 7.100  | 1.00 | 24.76 |
| ATOM | 3671 | O    | PRO | 152  | -1.610 | 17.920 | 7.428  | 1.00 | 25.13 |
| ATOM | 3672 | CB   | PRO | 152  | -3.017 | 15.430 | 8.925  | 1.00 | 26.39 |
| ATOM | 3673 | CG   | PRO | 152  | -1.977 | 15.825 | 9.910  | 1.00 | 27.66 |
| ATOM | 3674 | CD   | PRO | 152  | -0.765 | 15.087 | 9.397  | 1.00 | 27.22 |
| ATOM | 3675 | N    | PRO | 152A | -3.424 | 17.304 | 6.240  | 1.00 | 22.89 |
| ATOM | 3676 | CA   | PRO | 152A | -3.642 | 18.656 | 5.717  | 1.00 | 21.45 |
| ATOM | 3677 | C    | PRO | 152A | -4.019 | 19.579 | 6.878  | 1.00 | 20.40 |
| ATOM | 3678 | O    | PRO | 152A | -4.628 | 19.136 | 7.848  | 1.00 | 21.48 |
| ATOM | 3679 | CB   | PRO | 152A | -4.802 | 18.457 | 4.740  | 1.00 | 20.23 |
| ATOM | 3680 | CG   | PRO | 152A | -5.485 | 17.221 | 5.235  | 1.00 | 20.11 |
| ATOM | 3681 | CD   | PRO | 152A | -4.342 | 16.343 | 5.610  | 1.00 | 21.47 |
| ATOM | 3682 | N    | PRO | 152B | -3.627 | 20.861 | 6.822  | 1.00 | 19.54 |
| ATOM | 3683 | CA   | PRO | 152B | -3.130 | 21.633 | 5.682  | 1.00 | 20.04 |
| ATOM | 3684 | C    | PRO | 152B | -1.614 | 21.535 | 5.424  | 1.00 | 20.39 |
| ATOM | 3685 | O    | PRO | 152B | -0.980 | 22.533 | 5.054  | 1.00 | 20.71 |
| ATOM | 3686 | CB   | PRO | 152B | -3.534 | 23.053 | 6.059  | 1.00 | 19.55 |
| ATOM | 3687 | CG   | PRO | 152B | -3.275 | 23.066 | 7.514  | 1.00 | 17.27 |
| ATOM | 3688 | CD   | PRO | 152B | -3.874 | 21.753 | 7.969  | 1.00 | 18.19 |
| ATOM | 3689 | N    | PHE | 153  | -1.031 | 20.366 | 5.682  | 1.00 | 18.32 |
| ATOM | 3690 | CA   | PHE | 153  | 0.389  | 20.120 | 5.440  | 1.00 | 16.85 |
| ATOM | 3691 | C    | PHE | 153  | 1.321  | 21.248 | 5.902  | 1.00 | 17.00 |
| ATOM | 3692 | O    | PHE | 153  | 2.023  | 21.860 | 5.090  | 1.00 | 16.84 |
| ATOM | 3693 | CB   | PHE | 153  | 0.627  | 19.895 | 3.948  | 1.00 | 14.47 |
| ATOM | 3694 | CG   | PHE | 153  | -0.486 | 19.194 | 3.245  | 1.00 | 12.59 |
| ATOM | 3695 | CD1  | PHE | 153  | -1.423 | 19.921 | 2.521  | 1.00 | 11.93 |
| ATOM | 3696 | CD2  | PHE | 153  | -0.575 | 17.811 | 3.262  | 1.00 | 12.66 |
| ATOM | 3697 | CE1  | PHE | 153  | -2.429 | 19.281 | 1.819  | 1.00 | 11.58 |

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|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3698 | CE2  | PHE | 153 | -1.582 | 17.157 | 2.560  | 1.00 | 12.96 |
| ATOM | 3699 | CZ   | PHE | 153 | -2.511 | 17.893 | 1.836  | 1.00 | 12.43 |
| ATOM | 3700 | H    | PHE | 153 | -1.498 | 19.621 | 6.101  | 1.00 | 0.00  |
| ATOM | 3701 | N    | PRO | 154 | 1.349  | 21.535 | 7.205  | 1.00 | 16.98 |
| ATOM | 3702 | CA   | PRO | 154 | 2.224  | 22.607 | 7.685  | 1.00 | 18.46 |
| ATOM | 3703 | C    | PRO | 154 | 3.683  | 22.166 | 7.675  | 1.00 | 20.76 |
| ATOM | 3704 | O    | PRO | 154 | 3.964  | 20.976 | 7.796  | 1.00 | 23.06 |
| ATOM | 3705 | CB   | PRO | 154 | 1.728  | 22.814 | 9.106  | 1.00 | 18.11 |
| ATOM | 3706 | CG   | PRO | 154 | 1.398  | 21.404 | 9.538  | 1.00 | 17.22 |
| ATOM | 3707 | CD   | PRO | 154 | 0.690  | 20.838 | 8.325  | 1.00 | 17.21 |
| ATOM | 3708 | N    | LEU | 155 | 4.607  | 23.107 | 7.498  | 1.00 | 20.75 |
| ATOM | 3709 | CA   | LEU | 155 | 6.033  | 22.778 | 7.515  | 1.00 | 20.02 |
| ATOM | 3710 | C    | LEU | 155 | 6.431  | 22.537 | 8.969  | 1.00 | 20.39 |
| ATOM | 3711 | O    | LEU | 155 | 6.289  | 23.429 | 9.804  | 1.00 | 22.00 |
| ATOM | 3712 | CB   | LEU | 155 | 6.866  | 23.928 | 6.937  | 1.00 | 19.71 |
| ATOM | 3713 | CG   | LEU | 155 | 8.395  | 23.890 | 7.113  | 1.00 | 18.62 |
| ATOM | 3714 | CD1  | LEU | 155 | 8.985  | 22.667 | 6.439  | 1.00 | 18.68 |
| ATOM | 3715 | CD2  | LEU | 155 | 9.010  | 25.157 | 6.533  | 1.00 | 17.30 |
| ATOM | 3716 | H    | LEU | 155 | 4.308  | 24.025 | 7.345  | 1.00 | 0.00  |
| ATOM | 3717 | N    | LYS | 156 | 6.916  | 21.337 | 9.270  | 1.00 | 18.99 |
| ATOM | 3718 | CA   | LYS | 156 | 7.325  | 21.000 | 10.629 | 1.00 | 17.90 |
| ATOM | 3719 | C    | LYS | 156 | 8.836  | 21.054 | 10.807 | 1.00 | 17.45 |
| ATOM | 3720 | O    | LYS | 156 | 9.592  | 21.000 | 9.835  | 1.00 | 16.87 |
| ATOM | 3721 | CB   | LYS | 156 | 6.798  | 19.621 | 11.038 | 1.00 | 17.74 |
| ATOM | 3722 | CG   | LYS | 156 | 5.309  | 19.576 | 11.352 | 1.00 | 16.80 |
| ATOM | 3723 | CD   | LYS | 156 | 4.890  | 18.182 | 11.785 | 1.00 | 18.08 |
| ATOM | 3724 | CE   | LYS | 156 | 5.505  | 17.784 | 13.128 | 1.00 | 20.35 |
| ATOM | 3725 | NZ   | LYS | 156 | 5.344  | 16.329 | 13.460 | 1.00 | 20.97 |
| ATOM | 3726 | H    | LYS | 156 | 7.078  | 20.679 | 8.560  | 1.00 | 0.00  |
| ATOM | 3727 | HZ1  | LYS | 156 | 5.941  | 15.757 | 12.818 | 1.00 | 0.00  |
| ATOM | 3728 | HZ2  | LYS | 156 | 4.359  | 16.030 | 13.364 | 1.00 | 0.00  |
| ATOM | 3729 | HZ3  | LYS | 156 | 5.642  | 16.084 | 14.426 | 1.00 | 0.00  |
| ATOM | 3730 | N    | GLN | 157 | 9.258  | 21.123 | 12.067 | 1.00 | 18.39 |
| ATOM | 3731 | CA   | GLN | 157 | 10.664 | 21.210 | 12.450 | 1.00 | 19.27 |
| ATOM | 3732 | C    | GLN | 157 | 10.870 | 20.453 | 13.758 | 1.00 | 20.05 |
| ATOM | 3733 | O    | GLN | 157 | 9.923  | 20.256 | 14.517 | 1.00 | 20.91 |
| ATOM | 3734 | CB   | GLN | 157 | 11.018 | 22.675 | 12.712 | 1.00 | 19.96 |
| ATOM | 3735 | CG   | GLN | 157 | 10.229 | 23.272 | 13.895 | 1.00 | 19.36 |
| ATOM | 3736 | CD   | GLN | 157 | 10.516 | 24.742 | 14.160 | 1.00 | 20.05 |
| ATOM | 3737 | OE1  | GLN | 157 | 10.802 | 25.522 | 13.242 | 1.00 | 20.12 |
| ATOM | 3738 | NE2  | GLN | 157 | 10.418 | 25.132 | 15.420 | 1.00 | 19.86 |
| ATOM | 3739 | H    | GLN | 157 | 8.590  | 21.162 | 12.782 | 1.00 | 0.00  |
| ATOM | 3740 | HE21 | GLN | 157 | 10.162 | 24.470 | 16.090 | 1.00 | 0.00  |
| ATOM | 3741 | HE22 | GLN | 157 | 10.606 | 26.072 | 15.608 | 1.00 | 0.00  |
| ATOM | 3742 | N    | VAL | 158 | 12.110 | 20.076 | 14.044 | 1.00 | 19.79 |
| ATOM | 3743 | CA   | VAL | 158 | 12.424 | 19.388 | 15.286 | 1.00 | 19.85 |
| ATOM | 3744 | C    | VAL | 158 | 13.897 | 19.544 | 15.617 | 1.00 | 22.43 |
| ATOM | 3745 | O    | VAL | 158 | 14.737 | 19.550 | 14.716 | 1.00 | 24.62 |
| ATOM | 3746 | CB   | VAL | 158 | 12.078 | 17.898 | 15.224 | 1.00 | 18.99 |
| ATOM | 3747 | CG1  | VAL | 158 | 12.969 | 17.169 | 14.239 | 1.00 | 19.16 |
| ATOM | 3748 | CG2  | VAL | 158 | 12.218 | 17.303 | 16.587 | 1.00 | 20.14 |
| ATOM | 3749 | H    | VAL | 158 | 12.819 | 20.239 | 13.382 | 1.00 | 0.00  |
| ATOM | 3750 | N    | LYS | 159 | 14.206 | 19.729 | 16.896 | 1.00 | 24.32 |
| ATOM | 3751 | CA   | LYS | 159 | 15.596 | 19.870 | 17.318 | 1.00 | 26.22 |
| ATOM | 3752 | C    | LYS | 159 | 16.181 | 18.476 | 17.484 | 1.00 | 26.66 |
| ATOM | 3753 | O    | LYS | 159 | 15.661 | 17.669 | 18.256 | 1.00 | 27.72 |
| ATOM | 3754 | CB   | LYS | 159 | 15.702 | 20.640 | 18.640 | 1.00 | 28.05 |
| ATOM | 3755 | CG   | LYS | 159 | 17.143 | 20.892 | 19.093 | 1.00 | 30.96 |
| ATOM | 3756 | CD   | LYS | 159 | 17.236 | 21.509 | 20.494 | 1.00 | 33.80 |
| ATOM | 3757 | CE   | LYS | 159 | 16.838 | 22.992 | 20.539 | 1.00 | 35.50 |
| ATOM | 3758 | NZ   | LYS | 159 | 17.792 | 23.911 | 19.836 | 1.00 | 36.76 |
| ATOM | 3759 | H    | LYS | 159 | 13.474 | 19.763 | 17.547 | 1.00 | 0.00  |
| ATOM | 3760 | HZ1  | LYS | 159 | 17.817 | 23.689 | 18.819 | 1.00 | 0.00  |

|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3761 | HZ2  | LYS | 159 | 18.746 | 23.834 | 20.239 | 1.00 | 0.00  |
| ATOM | 3762 | HZ3  | LYS | 159 | 17.456 | 24.891 | 19.940 | 1.00 | 0.00  |
| ATOM | 3763 | N    | VAL | 160 | 17.252 | 18.192 | 16.756 | 1.00 | 25.77 |
| ATOM | 3764 | CA   | VAL | 160 | 17.894 | 16.890 | 16.820 | 1.00 | 25.19 |
| ATOM | 3765 | C    | VAL | 160 | 19.331 | 17.005 | 17.307 | 1.00 | 24.85 |
| ATOM | 3766 | O    | VAL | 160 | 20.053 | 17.922 | 16.917 | 1.00 | 24.58 |
| ATOM | 3767 | CB   | VAL | 160 | 17.892 | 16.190 | 15.441 | 1.00 | 25.80 |
| ATOM | 3768 | CG1  | VAL | 160 | 16.480 | 15.826 | 15.039 | 1.00 | 26.37 |
| ATOM | 3769 | CG2  | VAL | 160 | 18.531 | 17.086 | 14.391 | 1.00 | 24.77 |
| ATOM | 3770 | H    | VAL | 160 | 17.623 | 18.884 | 16.195 | 1.00 | 0.00  |
| ATOM | 3771 | N    | PRO | 161 | 19.736 | 16.116 | 18.230 | 1.00 | 24.60 |
| ATOM | 3772 | CA   | PRO | 161 | 21.093 | 16.101 | 18.783 | 1.00 | 23.63 |
| ATOM | 3773 | C    | PRO | 161 | 22.051 | 15.391 | 17.833 | 1.00 | 23.67 |
| ATOM | 3774 | O    | PRO | 161 | 21.764 | 14.277 | 17.407 | 1.00 | 23.91 |
| ATOM | 3775 | CB   | PRO | 161 | 20.911 | 15.303 | 20.071 | 1.00 | 23.61 |
| ATOM | 3776 | CG   | PRO | 161 | 19.834 | 14.326 | 19.709 | 1.00 | 21.45 |
| ATOM | 3777 | CD   | PRO | 161 | 18.854 | 15.205 | 18.989 | 1.00 | 23.62 |
| ATOM | 3778 | N    | ILE | 162 | 23.145 | 16.052 | 17.460 | 1.00 | 24.01 |
| ATOM | 3779 | CA   | ILE | 162 | 24.147 | 15.457 | 16.564 | 1.00 | 24.35 |
| ATOM | 3780 | C    | ILE | 162 | 24.814 | 14.283 | 17.270 | 1.00 | 26.36 |
| ATOM | 3781 | O    | ILE | 162 | 25.017 | 14.314 | 18.485 | 1.00 | 28.28 |
| ATOM | 3782 | CB   | ILE | 162 | 25.265 | 16.471 | 16.180 | 1.00 | 22.68 |
| ATOM | 3783 | CG1  | ILE | 162 | 24.772 | 17.459 | 15.128 | 1.00 | 22.47 |
| ATOM | 3784 | CG2  | ILE | 162 | 26.488 | 15.748 | 15.635 | 1.00 | 22.99 |
| ATOM | 3785 | H    | ILE | 162 | 23.295 | 16.977 | 17.753 | 1.00 | 0.00  |
| ATOM | 3786 | CD   | ILE | 162 | 24.562 | 16.840 | 13.773 | 1.00 | 23.92 |
| ATOM | 3787 | N    | MET | 163 | 25.171 | 13.259 | 16.508 | 1.00 | 26.92 |
| ATOM | 3788 | CA   | MET | 163 | 25.835 | 12.096 | 17.071 | 1.00 | 27.14 |
| ATOM | 3789 | C    | MET | 163 | 27.113 | 11.847 | 16.294 | 1.00 | 26.70 |
| ATOM | 3790 | O    | MET | 163 | 27.169 | 12.043 | 15.080 | 1.00 | 26.56 |
| ATOM | 3791 | CB   | MET | 163 | 24.935 | 10.863 | 17.018 | 1.00 | 28.49 |
| ATOM | 3792 | CG   | MET | 163 | 25.540 | 9.660  | 17.706 | 1.00 | 32.12 |
| ATOM | 3793 | SD   | MET | 163 | 24.403 | 8.288  | 17.898 | 1.00 | 35.49 |
| ATOM | 3794 | CE   | MET | 163 | 23.078 | 9.094  | 18.802 | 1.00 | 36.50 |
| ATOM | 3795 | H    | MET | 163 | 25.009 | 13.295 | 15.549 | 1.00 | 0.00  |
| ATOM | 3796 | N    | GLU | 164 | 28.147 | 11.441 | 17.016 | 1.00 | 26.10 |
| ATOM | 3797 | CA   | GLU | 164 | 29.447 | 11.168 | 16.437 | 1.00 | 25.57 |
| ATOM | 3798 | C    | GLU | 164 | 29.351 | 9.860  | 15.650 | 1.00 | 24.91 |
| ATOM | 3799 | O    | GLU | 164 | 28.704 | 8.910  | 16.101 | 1.00 | 24.54 |
| ATOM | 3800 | CB   | GLU | 164 | 30.464 | 11.078 | 17.574 | 1.00 | 26.32 |
| ATOM | 3801 | CG   | GLU | 164 | 31.889 | 11.396 | 17.193 | 1.00 | 27.94 |
| ATOM | 3802 | CD   | GLU | 164 | 32.647 | 10.184 | 16.731 | 1.00 | 29.60 |
| ATOM | 3803 | OE1  | GLU | 164 | 32.110 | 9.066  | 16.859 | 1.00 | 30.62 |
| ATOM | 3804 | OE2  | GLU | 164 | 33.787 | 10.340 | 16.245 | 1.00 | 31.23 |
| ATOM | 3805 | H    | GLU | 164 | 28.029 | 11.296 | 17.974 | 1.00 | 0.00  |
| ATOM | 3806 | N    | ASN | 165 | 29.965 | 9.826  | 14.467 | 1.00 | 24.44 |
| ATOM | 3807 | CA   | ASN | 165 | 29.936 | 8.643  | 13.598 | 1.00 | 23.80 |
| ATOM | 3808 | C    | ASN | 165 | 30.196 | 7.323  | 14.314 | 1.00 | 25.34 |
| ATOM | 3809 | O    | ASN | 165 | 29.352 | 6.441  | 14.297 | 1.00 | 24.57 |
| ATOM | 3810 | CB   | ASN | 165 | 30.925 | 8.779  | 12.427 | 1.00 | 21.73 |
| ATOM | 3811 | CG   | ASN | 165 | 30.386 | 9.630  | 11.280 | 1.00 | 19.60 |
| ATOM | 3812 | OD1  | ASN | 165 | 29.701 | 10.625 | 11.497 | 1.00 | 18.77 |
| ATOM | 3813 | ND2  | ASN | 165 | 30.725 | 9.255  | 10.056 | 1.00 | 17.38 |
| ATOM | 3814 | H    | ASN | 165 | 30.458 | 10.612 | 14.157 | 1.00 | 0.00  |
| ATOM | 3815 | HD21 | ASN | 165 | 31.292 | 8.468  | 9.911  | 1.00 | 0.00  |
| ATOM | 3816 | HD22 | ASN | 165 | 30.350 | 9.786  | 9.318  | 1.00 | 0.00  |
| ATOM | 3817 | N    | HIS | 166 | 31.339 | 7.210  | 14.985 | 1.00 | 29.08 |
| ATOM | 3818 | CA   | HIS | 166 | 31.720 | 5.981  | 15.690 | 1.00 | 31.78 |
| ATOM | 3819 | C    | HIS | 166 | 30.678 | 5.492  | 16.683 | 1.00 | 30.56 |
| ATOM | 3820 | O    | HIS | 166 | 30.415 | 4.291  | 16.779 | 1.00 | 29.97 |
| ATOM | 3821 | CB   | HIS | 166 | 33.062 | 6.161  | 16.396 | 1.00 | 37.52 |
| ATOM | 3822 | CG   | HIS | 166 | 34.184 | 6.513  | 15.470 | 1.00 | 44.81 |
| ATOM | 3823 | ND1  | HIS | 166 | 34.720 | 7.781  | 15.397 | 1.00 | 48.34 |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3824 | CD2 | HIS | 166 | 34.864 | 5.767  | 14.566 | 1.00 | 47.83 |
| ATOM | 3825 | CE1 | HIS | 166 | 35.678 | 7.805  | 14.487 | 1.00 | 50.35 |
| ATOM | 3826 | NE2 | HIS | 166 | 35.786 | 6.593  | 13.968 | 1.00 | 50.40 |
| ATOM | 3827 | H   | HIS | 166 | 31.909 | 8.003  | 15.080 | 1.00 | 0.00  |
| ATOM | 3828 | HD1 | HIS | 166 | 34.436 | 8.547  | 15.962 | 1.00 | 0.00  |
| ATOM | 3829 | HE2 | HIS | 166 | 36.430 | 6.307  | 13.297 | 1.00 | 0.00  |
| ATOM | 3830 | N   | ILE | 167 | 30.099 | 6.420  | 17.433 | 1.00 | 29.81 |
| ATOM | 3831 | CA  | ILE | 167 | 29.069 | 6.066  | 18.406 | 1.00 | 28.28 |
| ATOM | 3832 | C   | ILE | 167 | 27.817 | 5.604  | 17.659 | 1.00 | 28.58 |
| ATOM | 3833 | O   | ILE | 167 | 27.121 | 4.671  | 18.084 | 1.00 | 29.23 |
| ATOM | 3834 | CB  | ILE | 167 | 28.745 | 7.267  | 19.319 | 1.00 | 25.29 |
| ATOM | 3835 | CG1 | ILE | 167 | 29.918 | 7.516  | 20.263 | 1.00 | 22.49 |
| ATOM | 3836 | CG2 | ILE | 167 | 27.474 | 7.024  | 20.102 | 1.00 | 25.92 |
| ATOM | 3837 | H   | ILE | 167 | 30.420 | 7.343  | 17.333 | 1.00 | 0.00  |
| ATOM | 3838 | CD  | ILE | 167 | 30.225 | 6.346  | 21.150 | 1.00 | 19.13 |
| ATOM | 3839 | N   | CYS | 168 | 27.572 | 6.238  | 16.517 | 1.00 | 27.21 |
| ATOM | 3840 | CA  | CYS | 168 | 26.420 | 5.936  | 15.681 | 1.00 | 24.91 |
| ATOM | 3841 | C   | CYS | 168 | 26.536 | 4.595  | 14.978 | 1.00 | 23.89 |
| ATOM | 3842 | O   | CYS | 168 | 25.588 | 3.816  | 14.953 | 1.00 | 24.59 |
| ATOM | 3843 | CB  | CYS | 168 | 26.237 | 7.037  | 14.652 | 1.00 | 23.00 |
| ATOM | 3844 | SG  | CYS | 168 | 24.641 | 6.989  | 13.801 | 1.00 | 19.58 |
| ATOM | 3845 | H   | CYS | 168 | 28.172 | 6.967  | 16.256 | 1.00 | 0.00  |
| ATOM | 3846 | N   | ASP | 169 | 27.695 | 4.332  | 14.395 | 1.00 | 22.73 |
| ATOM | 3847 | CA  | ASP | 169 | 27.928 | 3.078  | 13.705 | 1.00 | 22.97 |
| ATOM | 3848 | C   | ASP | 169 | 27.700 | 1.939  | 14.700 | 1.00 | 23.84 |
| ATOM | 3849 | O   | ASP | 169 | 27.077 | 0.923  | 14.373 | 1.00 | 24.60 |
| ATOM | 3850 | CB  | ASP | 169 | 29.353 | 3.045  | 13.156 | 1.00 | 23.86 |
| ATOM | 3851 | CG  | ASP | 169 | 29.576 | 1.912  | 12.182 | 1.00 | 26.51 |
| ATOM | 3852 | OD1 | ASP | 169 | 28.592 | 1.453  | 11.569 | 1.00 | 27.87 |
| ATOM | 3853 | OD2 | ASP | 169 | 30.736 | 1.476  | 12.016 | 1.00 | 28.55 |
| ATOM | 3854 | H   | ASP | 169 | 28.392 | 4.986  | 14.412 | 1.00 | 0.00  |
| ATOM | 3855 | N   | ALA | 170 | 28.142 | 2.159  | 15.937 | 1.00 | 23.68 |
| ATOM | 3856 | CA  | ALA | 170 | 27.997 | 1.193  | 17.024 | 1.00 | 22.37 |
| ATOM | 3857 | C   | ALA | 170 | 26.545 | 0.776  | 17.184 | 1.00 | 20.80 |
| ATOM | 3858 | O   | ALA | 170 | 26.236 | -0.395 | 17.386 | 1.00 | 21.39 |
| ATOM | 3859 | CB  | ALA | 170 | 28.499 | 1.796  | 18.322 | 1.00 | 23.79 |
| ATOM | 3860 | H   | ALA | 170 | 28.622 | 2.995  | 16.114 | 1.00 | 0.00  |
| ATOM | 3861 | N   | LYS | 171 | 25.654 | 1.745  | 17.063 | 1.00 | 19.15 |
| ATOM | 3862 | CA  | LYS | 171 | 24.233 | 1.492  | 17.191 | 1.00 | 20.10 |
| ATOM | 3863 | C   | LYS | 171 | 23.716 | 0.607  | 16.055 | 1.00 | 19.94 |
| ATOM | 3864 | O   | LYS | 171 | 22.983 | -0.355 | 16.294 | 1.00 | 20.69 |
| ATOM | 3865 | CB  | LYS | 171 | 23.480 | 2.822  | 17.203 | 1.00 | 21.21 |
| ATOM | 3866 | CG  | LYS | 171 | 24.150 | 3.881  | 18.062 | 1.00 | 21.17 |
| ATOM | 3867 | CD  | LYS | 171 | 23.824 | 3.698  | 19.517 | 1.00 | 21.72 |
| ATOM | 3868 | CE  | LYS | 171 | 22.585 | 4.481  | 19.862 | 1.00 | 22.89 |
| ATOM | 3869 | NZ  | LYS | 171 | 22.867 | 5.945  | 19.819 | 1.00 | 23.93 |
| ATOM | 3870 | H   | LYS | 171 | 25.990 | 2.650  | 16.890 | 1.00 | 0.00  |
| ATOM | 3871 | HZ1 | LYS | 171 | 23.249 | 6.252  | 18.902 | 1.00 | 0.00  |
| ATOM | 3872 | HZ2 | LYS | 171 | 23.579 | 6.142  | 20.560 | 1.00 | 0.00  |
| ATOM | 3873 | HZ3 | LYS | 171 | 22.024 | 6.494  | 20.069 | 1.00 | 0.00  |
| ATOM | 3874 | N   | TYR | 172 | 24.122 | 0.908  | 14.825 | 1.00 | 19.08 |
| ATOM | 3875 | CA  | TYR | 172 | 23.658 | 0.135  | 13.678 | 1.00 | 19.28 |
| ATOM | 3876 | C   | TYR | 172 | 24.064 | -1.322 | 13.712 | 1.00 | 21.15 |
| ATOM | 3877 | O   | TYR | 172 | 23.418 | -2.172 | 13.092 | 1.00 | 22.03 |
| ATOM | 3878 | CB  | TYR | 172 | 24.045 | 0.797  | 12.358 | 1.00 | 17.33 |
| ATOM | 3879 | CG  | TYR | 172 | 23.017 | 1.813  | 11.915 | 1.00 | 16.92 |
| ATOM | 3880 | CD1 | TYR | 172 | 22.956 | 3.073  | 12.506 | 1.00 | 17.60 |
| ATOM | 3881 | CD2 | TYR | 172 | 22.078 | 1.505  | 10.935 | 1.00 | 16.62 |
| ATOM | 3882 | CE1 | TYR | 172 | 21.986 | 3.999  | 12.136 | 1.00 | 16.87 |
| ATOM | 3883 | CE2 | TYR | 172 | 21.109 | 2.423  | 10.560 | 1.00 | 17.13 |
| ATOM | 3884 | CZ  | TYR | 172 | 21.070 | 3.669  | 11.166 | 1.00 | 17.08 |
| ATOM | 3885 | OH  | TYR | 172 | 20.119 | 4.589  | 10.795 | 1.00 | 18.81 |
| ATOM | 3886 | H   | TYR | 172 | 24.723 | 1.676  | 14.705 | 1.00 | 0.00  |

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|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3887 | HH  | TYR | 172  | 19.627 | 4.211  | 10.073 | 1.00 | 0.00  |
| ATOM | 3888 | N   | HIS | 173  | 25.137 | -1.617 | 14.432 | 1.00 | 21.59 |
| ATOM | 3889 | CA  | HIS | 173  | 25.570 | -2.996 | 14.573 | 1.00 | 22.42 |
| ATOM | 3890 | C   | HIS | 173  | 24.785 | -3.636 | 15.708 | 1.00 | 24.81 |
| ATOM | 3891 | O   | HIS | 173  | 24.507 | -4.838 | 15.684 | 1.00 | 25.91 |
| ATOM | 3892 | CB  | HIS | 173  | 27.062 | -3.061 | 14.859 | 1.00 | 20.46 |
| ATOM | 3893 | CG  | HIS | 173  | 27.899 | -2.671 | 13.691 | 1.00 | 18.22 |
| ATOM | 3894 | ND1 | HIS | 173  | 28.356 | -3.585 | 12.769 | 1.00 | 17.81 |
| ATOM | 3895 | CD2 | HIS | 173  | 28.323 | -1.458 | 13.267 | 1.00 | 18.07 |
| ATOM | 3896 | CE1 | HIS | 173  | 29.022 | -2.949 | 11.822 | 1.00 | 18.52 |
| ATOM | 3897 | NE2 | HIS | 173  | 29.019 | -1.659 | 12.102 | 1.00 | 18.15 |
| ATOM | 3898 | H   | HIS | 173  | 25.644 | -0.875 | 14.824 | 1.00 | 0.00  |
| ATOM | 3899 | HD1 | HIS | 173  | 28.234 | -4.564 | 12.830 | 1.00 | 0.00  |
| ATOM | 3900 | HE2 | HIS | 173  | 29.511 | -0.946 | 11.624 | 1.00 | 0.00  |
| ATOM | 3901 | N   | LEU | 173A | 24.384 | -2.813 | 16.674 | 1.00 | 26.04 |
| ATOM | 3902 | CA  | LEU | 173A | 23.630 | -3.273 | 17.832 | 1.00 | 27.52 |
| ATOM | 3903 | C   | LEU | 173A | 22.260 | -3.809 | 17.431 | 1.00 | 27.26 |
| ATOM | 3904 | O   | LEU | 173A | 21.342 | -3.044 | 17.133 | 1.00 | 28.04 |
| ATOM | 3905 | CB  | LEU | 173A | 23.485 | -2.137 | 18.845 | 1.00 | 31.03 |
| ATOM | 3906 | CG  | LEU | 173A | 23.502 | -2.536 | 20.326 | 1.00 | 34.64 |
| ATOM | 3907 | CD1 | LEU | 173A | 23.961 | -1.346 | 21.165 | 1.00 | 35.28 |
| ATOM | 3908 | CD2 | LEU | 173A | 22.132 | -3.068 | 20.791 | 1.00 | 36.09 |
| ATOM | 3909 | H   | LEU | 173A | 24.608 | -1.858 | 16.631 | 1.00 | 0.00  |
| ATOM | 3910 | N   | GLY | 173B | 22.139 | -5.132 | 17.416 | 1.00 | 26.76 |
| ATOM | 3911 | CA  | GLY | 173B | 20.891 | -5.769 | 17.046 | 1.00 | 26.34 |
| ATOM | 3912 | C   | GLY | 173B | 20.935 | -6.315 | 15.632 | 1.00 | 26.87 |
| ATOM | 3913 | O   | GLY | 173B | 19.925 | -6.783 | 15.107 | 1.00 | 27.77 |
| ATOM | 3914 | H   | GLY | 173B | 22.933 | -5.677 | 17.604 | 1.00 | 0.00  |
| ATOM | 3915 | N   | ALA | 173C | 22.116 | -6.301 | 15.028 | 1.00 | 26.46 |
| ATOM | 3916 | CA  | ALA | 173C | 22.281 | -6.777 | 13.666 | 1.00 | 27.18 |
| ATOM | 3917 | C   | ALA | 173C | 23.362 | -7.849 | 13.583 | 1.00 | 28.08 |
| ATOM | 3918 | O   | ALA | 173C | 24.112 | -8.057 | 14.534 | 1.00 | 30.04 |
| ATOM | 3919 | CB  | ALA | 173C | 22.623 | -5.605 | 12.760 | 1.00 | 27.71 |
| ATOM | 3920 | H   | ALA | 173C | 22.935 | -5.987 | 15.464 | 1.00 | 0.00  |
| ATOM | 3921 | N   | TYR | 173D | 23.430 | -8.536 | 12.447 | 1.00 | 27.96 |
| ATOM | 3922 | CA  | TYR | 173D | 24.422 | -9.588 | 12.237 | 1.00 | 27.77 |
| ATOM | 3923 | C   | TYR | 173D | 25.723 | -9.049 | 11.653 | 1.00 | 26.96 |

|      |      |      |     |    |        |        |        |      |       |
|------|------|------|-----|----|--------|--------|--------|------|-------|
| ATOM | 2438 | HZ3  | LYS | 26 | 13.919 | 31.686 | 16.012 | 1.00 | 0.00  |
| ATOM | 2439 | N    | TRP | 27 | 12.642 | 29.272 | 8.099  | 1.00 | 30.07 |
| ATOM | 2440 | CA   | TRP | 27 | 13.527 | 28.493 | 7.250  | 1.00 | 26.81 |
| ATOM | 2441 | C    | TRP | 27 | 13.280 | 28.935 | 5.817  | 1.00 | 26.48 |
| ATOM | 2442 | O    | TRP | 27 | 12.693 | 28.212 | 5.022  | 1.00 | 26.57 |
| ATOM | 2443 | CB   | TRP | 27 | 13.235 | 27.001 | 7.430  | 1.00 | 24.02 |
| ATOM | 2444 | CG   | TRP | 27 | 13.038 | 26.596 | 8.866  | 1.00 | 20.50 |
| ATOM | 2445 | CD1  | TRP | 27 | 11.860 | 26.266 | 9.461  | 1.00 | 21.21 |
| ATOM | 2446 | CD2  | TRP | 27 | 14.045 | 26.475 | 9.880  | 1.00 | 19.98 |
| ATOM | 2447 | NE1  | TRP | 27 | 12.064 | 25.943 | 10.782 | 1.00 | 19.35 |
| ATOM | 2448 | CE2  | TRP | 27 | 13.395 | 26.059 | 11.066 | 1.00 | 18.90 |
| ATOM | 2449 | CE3  | TRP | 27 | 15.431 | 26.676 | 9.905  | 1.00 | 19.98 |
| ATOM | 2450 | CZ2  | TRP | 27 | 14.081 | 25.837 | 12.260 | 1.00 | 17.99 |
| ATOM | 2451 | CZ3  | TRP | 27 | 16.116 | 26.458 | 11.096 | 1.00 | 19.13 |
| ATOM | 2452 | CH2  | TRP | 27 | 15.437 | 26.039 | 12.257 | 1.00 | 19.26 |
| ATOM | 2453 | H    | TRP | 27 | 11.727 | 29.436 | 7.831  | 1.00 | 0.00  |
| ATOM | 2454 | HE1  | TRP | 27 | 11.390 | 25.696 | 11.450 | 1.00 | 0.00  |
| ATOM | 2455 | N    | PRO | 28 | 13.751 | 30.134 | 5.463  | 1.00 | 26.55 |
| ATOM | 2456 | CA   | PRO | 28 | 13.587 | 30.706 | 4.123  | 1.00 | 26.76 |
| ATOM | 2457 | C    | PRO | 28 | 14.279 | 29.954 | 3.000  | 1.00 | 26.36 |
| ATOM | 2458 | O    | PRO | 28 | 14.131 | 30.321 | 1.837  | 1.00 | 27.58 |
| ATOM | 2459 | CB   | PRO | 28 | 14.165 | 32.111 | 4.282  | 1.00 | 26.65 |
| ATOM | 2460 | CG   | PRO | 28 | 15.250 | 31.902 | 5.278  | 1.00 | 27.42 |
| ATOM | 2461 | CD   | PRO | 28 | 14.581 | 31.011 | 6.304  | 1.00 | 26.84 |
| ATOM | 2462 | N    | TRP | 29 | 15.035 | 28.916 | 3.345  | 1.00 | 25.45 |
| ATOM | 2463 | CA   | TRP | 29 | 15.750 | 28.129 | 2.341  | 1.00 | 25.13 |
| ATOM | 2464 | C    | TRP | 29 | 15.098 | 26.789 | 1.994  | 1.00 | 24.78 |
| ATOM | 2465 | O    | TRP | 29 | 15.530 | 26.120 | 1.049  | 1.00 | 25.95 |
| ATOM | 2466 | CB   | TRP | 29 | 17.194 | 27.884 | 2.784  | 1.00 | 24.26 |
| ATOM | 2467 | CG   | TRP | 29 | 17.310 | 27.230 | 4.132  | 1.00 | 22.84 |
| ATOM | 2468 | CD1  | TRP | 29 | 17.081 | 25.915 | 4.435  | 1.00 | 22.16 |
| ATOM | 2469 | CD2  | TRP | 29 | 17.669 | 27.869 | 5.360  | 1.00 | 22.18 |
| ATOM | 2470 | NE1  | TRP | 29 | 17.270 | 25.701 | 5.776  | 1.00 | 22.28 |
| ATOM | 2471 | CE2  | TRP | 29 | 17.632 | 26.882 | 6.370  | 1.00 | 22.66 |
| ATOM | 2472 | CE3  | TRP | 29 | 18.021 | 29.182 | 5.706  | 1.00 | 20.83 |
| ATOM | 2473 | CZ2  | TRP | 29 | 17.930 | 27.167 | 7.704  | 1.00 | 22.91 |
| ATOM | 2474 | CZ3  | TRP | 29 | 18.317 | 29.467 | 7.030  | 1.00 | 20.78 |
| ATOM | 2475 | CH2  | TRP | 29 | 18.269 | 28.462 | 8.014  | 1.00 | 23.06 |
| ATOM | 2476 | H    | TRP | 29 | 15.119 | 28.665 | 4.279  | 1.00 | 0.00  |
| ATOM | 2477 | HE1  | TRP | 29 | 17.126 | 24.846 | 6.245  | 1.00 | 0.00  |
| ATOM | 2478 | N    | GLN | 30 | 14.087 | 26.395 | 2.770  | 1.00 | 22.56 |
| ATOM | 2479 | CA   | GLN | 30 | 13.378 | 25.132 | 2.569  | 1.00 | 19.79 |
| ATOM | 2480 | C    | GLN | 30 | 12.780 | 25.071 | 1.168  | 1.00 | 19.70 |
| ATOM | 2481 | O    | GLN | 30 | 12.359 | 26.096 | 0.617  | 1.00 | 21.33 |
| ATOM | 2482 | CB   | GLN | 30 | 12.277 | 24.981 | 3.621  | 1.00 | 18.14 |
| ATOM | 2483 | CG   | GLN | 30 | 11.552 | 23.651 | 3.602  | 1.00 | 16.12 |
| ATOM | 2484 | CD   | GLN | 30 | 12.447 | 22.491 | 3.952  | 1.00 | 14.29 |
| ATOM | 2485 | OE1  | GLN | 30 | 12.496 | 21.497 | 3.231  | 1.00 | 15.76 |
| ATOM | 2486 | NE2  | GLN | 30 | 13.159 | 22.604 | 5.063  | 1.00 | 11.06 |
| ATOM | 2487 | H    | GLN | 30 | 13.745 | 26.996 | 3.457  | 1.00 | 0.00  |
| ATOM | 2488 | HE21 | GLN | 30 | 13.100 | 23.413 | 5.605  | 1.00 | 0.00  |
| ATOM | 2489 | HE22 | GLN | 30 | 13.720 | 21.832 | 5.270  | 1.00 | 0.00  |
| ATOM | 2490 | N    | VAL | 31 | 12.759 | 23.876 | 0.592  | 1.00 | 18.32 |
| ATOM | 2491 | CA   | VAL | 31 | 12.228 | 23.678 | -0.750 | 1.00 | 17.12 |
| ATOM | 2492 | C    | VAL | 31 | 11.439 | 22.375 | -0.845 | 1.00 | 16.16 |
| ATOM | 2493 | O    | VAL | 31 | 11.690 | 21.430 | -0.092 | 1.00 | 16.44 |
| ATOM | 2494 | CB   | VAL | 31 | 13.375 | 23.690 | -1.799 | 1.00 | 16.99 |
| ATOM | 2495 | CG1  | VAL | 31 | 12.932 | 23.065 | -3.107 | 1.00 | 17.45 |
| ATOM | 2496 | CG2  | VAL | 31 | 13.832 | 25.119 | -2.052 | 1.00 | 18.64 |
| ATOM | 2497 | H    | VAL | 31 | 13.122 | 23.086 | 1.052  | 1.00 | 0.00  |
| ATOM | 2498 | N    | SER | 32 | 10.445 | 22.367 | -1.728 | 1.00 | 14.09 |
| ATOM | 2499 | CA   | SER | 32 | 9.609  | 21.205 | -1.971 | 1.00 | 13.42 |
| ATOM | 2500 | C    | SER | 32 | 9.792  | 20.816 | -3.428 | 1.00 | 13.80 |

|      |      |      |     |     |        |        |         |      |       |
|------|------|------|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2501 | O    | SER | 32  | 9.605  | 21.649 | -4.313  | 1.00 | 15.20 |
| ATOM | 2502 | CB   | SER | 32  | 8.141  | 21.544 | -1.716  | 1.00 | 13.19 |
| ATOM | 2503 | OG   | SER | 32  | 7.288  | 20.484 | -2.125  | 1.00 | 12.32 |
| ATOM | 2504 | H    | SER | 32  | 10.255 | 23.191 | -2.219  | 1.00 | 0.00  |
| ATOM | 2505 | HG   | SER | 32  | 6.372  | 20.719 | -1.909  | 1.00 | 0.00  |
| ATOM | 2506 | N    | LEU | 33  | 10.233 | 19.585 | -3.667  | 1.00 | 13.20 |
| ATOM | 2507 | CA   | LEU | 33  | 10.428 | 19.085 | -5.020  | 1.00 | 13.21 |
| ATOM | 2508 | C    | LEU | 33  | 9.149  | 18.369 | -5.394  | 1.00 | 15.47 |
| ATOM | 2509 | O    | LEU | 33  | 8.661  | 17.535 | -4.622  | 1.00 | 16.81 |
| ATOM | 2510 | CB   | LEU | 33  | 11.604 | 18.111 | -5.085  | 1.00 | 12.12 |
| ATOM | 2511 | CG   | LEU | 33  | 13.004 | 18.616 | -4.739  | 1.00 | 11.95 |
| ATOM | 2512 | CD1  | LEU | 33  | 14.048 | 17.626 | -5.256  | 1.00 | 10.82 |
| ATOM | 2513 | CD2  | LEU | 33  | 13.227 | 19.984 | -5.353  | 1.00 | 11.27 |
| ATOM | 2514 | H    | LEU | 33  | 10.429 | 19.005 | -2.915  | 1.00 | 0.00  |
| ATOM | 2515 | N    | ARG | 34  | 8.618  | 18.671 | -6.575  | 1.00 | 16.91 |
| ATOM | 2516 | CA   | ARG | 34  | 7.370  | 18.069 | -7.031  | 1.00 | 19.06 |
| ATOM | 2517 | C    | ARG | 34  | 7.516  | 17.201 | -8.280  | 1.00 | 21.65 |
| ATOM | 2518 | O    | ARG | 34  | 8.478  | 17.342 | -9.036  | 1.00 | 23.43 |
| ATOM | 2519 | CB   | ARG | 34  | 6.354  | 19.167 | -7.340  | 1.00 | 17.58 |
| ATOM | 2520 | CG   | ARG | 34  | 6.261  | 20.267 | -6.318  | 1.00 | 16.22 |
| ATOM | 2521 | CD   | ARG | 34  | 5.594  | 19.814 | -5.036  | 1.00 | 16.92 |
| ATOM | 2522 | NE   | ARG | 34  | 5.360  | 20.971 | -4.173  | 1.00 | 18.23 |
| ATOM | 2523 | CZ   | ARG | 34  | 4.220  | 21.660 | -4.115  | 1.00 | 17.31 |
| ATOM | 2524 | NH1  | ARG | 34  | 3.171  | 21.309 | -4.854  | 1.00 | 16.04 |
| ATOM | 2525 | NH2  | ARG | 34  | 4.132  | 22.717 | -3.315  | 1.00 | 18.61 |
| ATOM | 2526 | H    | ARG | 34  | 9.083  | 19.302 | -7.162  | 1.00 | 0.00  |
| ATOM | 2527 | HE   | ARG | 34  | 6.127  | 21.197 | -3.616  | 1.00 | 0.00  |
| ATOM | 2528 | HH11 | ARG | 34  | 3.136  | 20.499 | -5.443  | 1.00 | 0.00  |
| ATOM | 2529 | HH12 | ARG | 34  | 2.344  | 21.904 | -4.839  | 1.00 | 0.00  |
| ATOM | 2530 | HH21 | ARG | 34  | 4.824  | 23.118 | -2.714  | 1.00 | 0.00  |
| ATOM | 2531 | HH22 | ARG | 34  | 3.269  | 23.270 | -3.296  | 1.00 | 0.00  |
| ATOM | 2532 | N    | VAL | 35  | 6.544  | 16.311 | -8.485  | 1.00 | 23.39 |
| ATOM | 2533 | CA   | VAL | 35  | 6.487  | 15.439 | -9.656  | 1.00 | 25.24 |
| ATOM | 2534 | C    | VAL | 35  | 5.079  | 15.486 | -10.208 | 1.00 | 29.75 |
| ATOM | 2535 | O    | VAL | 35  | 4.102  | 15.568 | -9.451  | 1.00 | 29.19 |
| ATOM | 2536 | CB   | VAL | 35  | 6.809  | 13.970 | -9.354  | 1.00 | 22.92 |
| ATOM | 2537 | CG1  | VAL | 35  | 8.289  | 13.756 | -9.358  | 1.00 | 24.74 |
| ATOM | 2538 | CG2  | VAL | 35  | 6.200  | 13.546 | -8.039  | 1.00 | 22.83 |
| ATOM | 2539 | H    | VAL | 35  | 5.841  | 16.248 | -7.804  | 1.00 | 0.00  |
| ATOM | 2540 | N    | HIS | 36  | 4.992  | 15.403 | -11.532 | 1.00 | 34.90 |
| ATOM | 2541 | CA   | HIS | 36  | 3.728  | 15.445 | -12.251 | 1.00 | 39.85 |
| ATOM | 2542 | C    | HIS | 36  | 2.504  | 14.880 | -11.533 | 1.00 | 40.09 |
| ATOM | 2543 | O    | HIS | 36  | 1.666  | 15.649 | -11.079 | 1.00 | 42.12 |
| ATOM | 2544 | CB   | HIS | 36  | 3.873  | 14.865 | -13.670 | 1.00 | 48.03 |
| ATOM | 2545 | CG   | HIS | 36  | 4.247  | 13.407 | -13.722 | 1.00 | 56.59 |
| ATOM | 2546 | ND1  | HIS | 36  | 5.437  | 12.911 | -13.226 | 1.00 | 59.53 |
| ATOM | 2547 | CD2  | HIS | 36  | 3.598  | 12.344 | -14.263 | 1.00 | 59.06 |
| ATOM | 2548 | CE1  | HIS | 36  | 5.505  | 11.611 | -13.459 | 1.00 | 60.32 |
| ATOM | 2549 | NE2  | HIS | 36  | 4.403  | 11.243 | -14.088 | 1.00 | 60.67 |
| ATOM | 2550 | H    | HIS | 36  | 5.840  | 15.437 | -12.013 | 1.00 | 0.00  |
| ATOM | 2551 | HD1  | HIS | 36  | 6.202  | 13.362 | -12.790 | 1.00 | 0.00  |
| ATOM | 2552 | HE2  | HIS | 36  | 4.194  | 10.338 | -14.407 | 1.00 | 0.00  |
| ATOM | 2553 | N    | GLY | 37  | 2.403  | 13.559 | -11.408 | 1.00 | 38.78 |
| ATOM | 2554 | CA   | GLY | 37  | 1.248  | 12.964 | -10.743 | 1.00 | 38.47 |
| ATOM | 2555 | C    | GLY | 37  | -0.096 | 13.228 | -11.422 | 1.00 | 36.88 |
| ATOM | 2556 | O    | GLY | 37  | -0.129 | 13.644 | -12.580 | 1.00 | 37.63 |
| ATOM | 2557 | H    | GLY | 37  | 3.105  | 12.971 | -11.713 | 1.00 | 0.00  |
| ATOM | 2558 | N    | PRO | 37A | -1.226 | 12.954 | -10.740 | 1.00 | 35.09 |
| ATOM | 2559 | CA   | PRO | 37A | -2.480 | 13.700 | -10.906 | 1.00 | 33.69 |
| ATOM | 2560 | C    | PRO | 37A | -2.324 | 15.161 | -10.497 | 1.00 | 32.82 |
| ATOM | 2561 | O    | PRO | 37A | -3.130 | 16.012 | -10.865 | 1.00 | 32.88 |
| ATOM | 2562 | CB   | PRO | 37A | -3.433 | 12.973 | -9.962  | 1.00 | 33.08 |
| ATOM | 2563 | CG   | PRO | 37A | -2.909 | 11.584 | -9.955  | 1.00 | 33.35 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2564 | CD  | PRO | 37A | -1.429 | 11.804 | -9.845  | 1.00 | 34.14 |
| ATOM | 2565 | N   | TYR | 37B | -1.309 | 15.429 | -9.686  | 1.00 | 31.45 |
| ATOM | 2566 | CA  | TYR | 37B | -1.022 | 16.776 | -9.225  | 1.00 | 30.81 |
| ATOM | 2567 | C   | TYR | 37B | 0.453  | 16.838 | -8.859  | 1.00 | 31.27 |
| ATOM | 2568 | O   | TYR | 37B | 1.084  | 15.809 | -8.581  | 1.00 | 32.71 |
| ATOM | 2569 | CB  | TYR | 37B | -1.881 | 17.142 | -8.011  | 1.00 | 28.47 |
| ATOM | 2570 | CG  | TYR | 37B | -1.623 | 16.309 | -6.772  | 1.00 | 28.52 |
| ATOM | 2571 | CD1 | TYR | 37B | -0.927 | 16.835 | -5.685  | 1.00 | 28.66 |
| ATOM | 2572 | CD2 | TYR | 37B | -2.107 | 15.008 | -6.670  | 1.00 | 29.80 |
| ATOM | 2573 | CE1 | TYR | 37B | -0.726 | 16.082 | -4.527  | 1.00 | 28.84 |
| ATOM | 2574 | CE2 | TYR | 37B | -1.912 | 14.249 | -5.513  | 1.00 | 29.05 |
| ATOM | 2575 | CZ  | TYR | 37B | -1.225 | 14.793 | -4.450  | 1.00 | 28.75 |
| ATOM | 2576 | OH  | TYR | 37B | -1.064 | 14.054 | -3.299  | 1.00 | 30.25 |
| ATOM | 2577 | H   | TYR | 37B | -0.674 | 14.741 | -9.401  | 1.00 | 0.00  |
| ATOM | 2578 | HH  | TYR | 37B | -0.442 | 14.569 | -2.765  | 1.00 | 0.00  |
| ATOM | 2579 | N   | TRP | 38  | 1.002  | 18.045 | -8.875  | 1.00 | 29.57 |
| ATOM | 2580 | CA  | TRP | 38  | 2.395  | 18.258 | -8.535  | 1.00 | 27.83 |
| ATOM | 2581 | C   | TRP | 38  | 2.636  | 17.823 | -7.102  | 1.00 | 27.67 |
| ATOM | 2582 | O   | TRP | 38  | 2.667  | 18.633 | -6.172  | 1.00 | 27.98 |
| ATOM | 2583 | CB  | TRP | 38  | 2.738  | 19.719 | -8.756  | 1.00 | 27.58 |
| ATOM | 2584 | CG  | TRP | 38  | 2.673  | 20.045 | -10.193 | 1.00 | 27.51 |
| ATOM | 2585 | CD1 | TRP | 38  | 1.665  | 20.691 | -10.844 | 1.00 | 26.98 |
| ATOM | 2586 | CD2 | TRP | 38  | 3.627  | 19.665 | -11.194 | 1.00 | 27.86 |
| ATOM | 2587 | NE1 | TRP | 38  | 1.927  | 20.728 | -12.192 | 1.00 | 27.54 |
| ATOM | 2588 | CE2 | TRP | 38  | 3.128  | 20.109 | -12.434 | 1.00 | 27.71 |
| ATOM | 2589 | CE3 | TRP | 38  | 4.858  | 18.990 | -11.161 | 1.00 | 27.01 |
| ATOM | 2590 | CZ2 | TRP | 38  | 3.817  | 19.899 | -13.638 | 1.00 | 27.95 |
| ATOM | 2591 | CZ3 | TRP | 38  | 5.539  | 18.784 | -12.357 | 1.00 | 27.43 |
| ATOM | 2592 | CH2 | TRP | 38  | 5.016  | 19.238 | -13.579 | 1.00 | 27.02 |
| ATOM | 2593 | H   | TRP | 38  | 0.448  | 18.808 | -9.123  | 1.00 | 0.00  |
| ATOM | 2594 | HE1 | TRP | 38  | 1.328  | 21.111 | -12.868 | 1.00 | 0.00  |
| ATOM | 2595 | N   | MET | 39  | 2.836  | 16.525 | -6.955  | 1.00 | 27.45 |
| ATOM | 2596 | CA  | MET | 39  | 3.039  | 15.888 | -5.674  | 1.00 | 28.88 |
| ATOM | 2597 | C   | MET | 39  | 4.417  | 16.177 | -5.078  | 1.00 | 28.83 |
| ATOM | 2598 | O   | MET | 39  | 5.414  | 16.207 | -5.802  | 1.00 | 30.54 |
| ATOM | 2599 | CB  | MET | 39  | 2.873  | 14.391 | -5.886  | 1.00 | 31.85 |
| ATOM | 2600 | CG  | MET | 39  | 2.399  | 13.616 | -4.692  | 1.00 | 34.61 |
| ATOM | 2601 | SD  | MET | 39  | 2.224  | 11.903 | -5.183  | 1.00 | 37.58 |
| ATOM | 2602 | CE  | MET | 39  | 1.325  | 12.088 | -6.775  | 1.00 | 35.07 |
| ATOM | 2603 | H   | MET | 39  | 2.895  | 15.993 | -7.783  | 1.00 | 0.00  |
| ATOM | 2604 | N   | HIS | 40  | 4.465  | 16.430 | -3.770  | 1.00 | 25.91 |
| ATOM | 2605 | CA  | HIS | 40  | 5.732  | 16.680 | -3.077  | 1.00 | 23.53 |
| ATOM | 2606 | C   | HIS | 40  | 6.411  | 15.335 | -2.854  | 1.00 | 22.49 |
| ATOM | 2607 | O   | HIS | 40  | 5.818  | 14.460 | -2.223  | 1.00 | 24.35 |
| ATOM | 2608 | CB  | HIS | 40  | 5.482  | 17.342 | -1.709  | 1.00 | 21.80 |
| ATOM | 2609 | CG  | HIS | 40  | 6.626  | 17.214 | -0.743  | 1.00 | 19.85 |
| ATOM | 2610 | ND1 | HIS | 40  | 7.636  | 18.144 | -0.655  | 1.00 | 19.82 |
| ATOM | 2611 | CD2 | HIS | 40  | 6.925  | 16.252 | 0.165   | 1.00 | 19.92 |
| ATOM | 2612 | CE1 | HIS | 40  | 8.511  | 17.765 | 0.259   | 1.00 | 19.50 |
| ATOM | 2613 | NE2 | HIS | 40  | 8.104  | 16.618 | 0.771   | 1.00 | 19.97 |
| ATOM | 2614 | H   | HIS | 40  | 3.627  | 16.493 | -3.265  | 1.00 | 0.00  |
| ATOM | 2615 | HD1 | HIS | 40  | 7.692  | 18.959 | -1.198  | 1.00 | 0.00  |
| ATOM | 2616 | HE2 | HIS | 40  | 8.620  | 16.094 | 1.430   | 1.00 | 0.00  |
| ATOM | 2617 | N   | PHE | 41  | 7.641  | 15.163 | -3.335  | 1.00 | 19.65 |
| ATOM | 2618 | CA  | PHE | 41  | 8.345  | 13.896 | -3.122  | 1.00 | 17.53 |
| ATOM | 2619 | C   | PHE | 41  | 9.585  | 14.014 | -2.227  | 1.00 | 16.64 |
| ATOM | 2620 | O   | PHE | 41  | 10.013 | 13.045 | -1.599  | 1.00 | 15.87 |
| ATOM | 2621 | CB  | PHE | 41  | 8.672  | 13.190 | -4.461  | 1.00 | 16.21 |
| ATOM | 2622 | CG  | PHE | 41  | 9.729  | 13.875 | -5.302  | 1.00 | 15.02 |
| ATOM | 2623 | CD1 | PHE | 41  | 11.068 | 13.529 | -5.179  | 1.00 | 13.68 |
| ATOM | 2624 | CD2 | PHE | 41  | 9.382  | 14.833 | -6.243  | 1.00 | 15.50 |
| ATOM | 2625 | CE1 | PHE | 41  | 12.040 | 14.125 | -5.977  | 1.00 | 13.28 |
| ATOM | 2626 | CE2 | PHE | 41  | 10.357 | 15.432 | -7.047  | 1.00 | 15.21 |

|      |      |     |     |    |        |        |        |      |       |
|------|------|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 2627 | CZ  | PHE | 41 | 11.686 | 15.075 | -6.910 | 1.00 | 13.41 |
| ATOM | 2628 | H   | PHE | 41 | 8.037  | 15.900 | -3.847 | 1.00 | 0.00  |
| ATOM | 2629 | N   | CYS | 42 | 10.108 | 15.226 | -2.106 | 1.00 | 16.41 |
| ATOM | 2630 | CA  | CYS | 42 | 11.295 | 15.468 | -1.305 | 1.00 | 15.51 |
| ATOM | 2631 | C   | CYS | 42 | 11.450 | 16.939 | -0.995 | 1.00 | 16.13 |
| ATOM | 2632 | O   | CYS | 42 | 10.766 | 17.782 | -1.577 | 1.00 | 17.43 |
| ATOM | 2633 | CB  | CYS | 42 | 12.527 | 15.022 | -2.072 | 1.00 | 13.97 |
| ATOM | 2634 | SG  | CYS | 42 | 12.861 | 13.250 | -1.978 | 1.00 | 13.42 |
| ATOM | 2635 | H   | CYS | 42 | 9.721  | 15.976 | -2.597 | 1.00 | 0.00  |
| ATOM | 2636 | N   | GLY | 43 | 12.358 | 17.239 | -0.080 | 1.00 | 15.27 |
| ATOM | 2637 | CA  | GLY | 43 | 12.609 | 18.612 | 0.290  | 1.00 | 15.57 |
| ATOM | 2638 | C   | GLY | 43 | 13.929 | 18.982 | -0.330 | 1.00 | 17.30 |
| ATOM | 2639 | O   | GLY | 43 | 14.477 | 18.211 | -1.122 | 1.00 | 19.14 |
| ATOM | 2640 | H   | GLY | 43 | 12.929 | 16.526 | 0.285  | 1.00 | 0.00  |
| ATOM | 2641 | N   | GLY | 44 | 14.447 | 20.146 | 0.040  | 1.00 | 17.05 |
| ATOM | 2642 | CA  | GLY | 44 | 15.721 | 20.605 | -0.485 | 1.00 | 17.02 |
| ATOM | 2643 | C   | GLY | 44 | 16.006 | 21.969 | 0.100  | 1.00 | 17.99 |
| ATOM | 2644 | O   | GLY | 44 | 15.235 | 22.446 | 0.935  | 1.00 | 19.89 |
| ATOM | 2645 | H   | GLY | 44 | 13.969 | 20.713 | 0.677  | 1.00 | 0.00  |
| ATOM | 2646 | N   | SER | 45 | 17.105 | 22.594 | -0.297 | 1.00 | 17.11 |
| ATOM | 2647 | CA  | SER | 45 | 17.423 | 23.918 | 0.213  | 1.00 | 17.01 |
| ATOM | 2648 | C   | SER | 45 | 18.030 | 24.784 | -0.866 | 1.00 | 17.61 |
| ATOM | 2649 | O   | SER | 45 | 18.636 | 24.278 | -1.814 | 1.00 | 19.51 |
| ATOM | 2650 | CB  | SER | 45 | 18.381 | 23.823 | 1.391  | 1.00 | 17.98 |
| ATOM | 2651 | OG  | SER | 45 | 19.564 | 23.162 | 1.003  | 1.00 | 21.12 |
| ATOM | 2652 | H   | SER | 45 | 17.735 | 22.124 | -0.887 | 1.00 | 0.00  |
| ATOM | 2653 | HG  | SER | 45 | 20.281 | 23.346 | 1.622  | 1.00 | 0.00  |
| ATOM | 2654 | N   | LEU | 46 | 17.826 | 26.087 | -0.739 | 1.00 | 17.02 |
| ATOM | 2655 | CA  | LEU | 46 | 18.359 | 27.052 | -1.689 | 1.00 | 17.24 |
| ATOM | 2656 | C   | LEU | 46 | 19.774 | 27.389 | -1.223 | 1.00 | 19.59 |
| ATOM | 2657 | O   | LEU | 46 | 19.949 | 28.114 | -0.245 | 1.00 | 21.65 |
| ATOM | 2658 | CB  | LEU | 46 | 17.490 | 28.302 | -1.658 | 1.00 | 14.31 |
| ATOM | 2659 | CG  | LEU | 46 | 17.444 | 29.197 | -2.882 | 1.00 | 10.66 |
| ATOM | 2660 | CD1 | LEU | 46 | 16.885 | 28.416 | -4.041 | 1.00 | 8.44  |
| ATOM | 2661 | CD2 | LEU | 46 | 16.562 | 30.389 | -2.572 | 1.00 | 9.92  |
| ATOM | 2662 | H   | LEU | 46 | 17.269 | 26.385 | 0.007  | 1.00 | 0.00  |
| ATOM | 2663 | N   | ILE | 47 | 20.789 | 26.839 | -1.882 | 1.00 | 20.63 |
| ATOM | 2664 | CA  | ILE | 47 | 22.166 | 27.108 | -1.475 | 1.00 | 21.59 |
| ATOM | 2665 | C   | ILE | 47 | 22.809 | 28.261 | -2.243 | 1.00 | 26.00 |
| ATOM | 2666 | O   | ILE | 47 | 23.941 | 28.657 | -1.956 | 1.00 | 28.12 |
| ATOM | 2667 | CB  | ILE | 47 | 23.040 | 25.860 | -1.609 | 1.00 | 18.83 |
| ATOM | 2668 | CG1 | ILE | 47 | 23.199 | 25.474 | -3.082 | 1.00 | 17.78 |
| ATOM | 2669 | CG2 | ILE | 47 | 22.426 | 24.729 | -0.812 | 1.00 | 19.00 |
| ATOM | 2670 | H   | ILE | 47 | 20.574 | 26.259 | -2.650 | 1.00 | 0.00  |
| ATOM | 2671 | CD  | ILE | 47 | 24.117 | 24.279 | -3.329 | 1.00 | 15.97 |
| ATOM | 2672 | N   | HIS | 48 | 22.063 | 28.812 | -3.197 | 1.00 | 28.50 |
| ATOM | 2673 | CA  | HIS | 48 | 22.507 | 29.919 | -4.048 | 1.00 | 29.64 |
| ATOM | 2674 | C   | HIS | 48 | 21.244 | 30.318 | -4.802 | 1.00 | 30.24 |
| ATOM | 2675 | O   | HIS | 48 | 20.396 | 29.470 | -5.071 | 1.00 | 30.81 |
| ATOM | 2676 | CB  | HIS | 48 | 23.581 | 29.422 | -5.026 | 1.00 | 31.70 |
| ATOM | 2677 | CG  | HIS | 48 | 24.036 | 30.448 | -6.018 | 1.00 | 33.16 |
| ATOM | 2678 | ND1 | HIS | 48 | 25.240 | 31.110 | -5.904 | 1.00 | 34.00 |
| ATOM | 2679 | CD2 | HIS | 48 | 23.466 | 30.901 | -7.161 | 1.00 | 32.66 |
| ATOM | 2680 | CE1 | HIS | 48 | 25.392 | 31.925 | -6.932 | 1.00 | 35.23 |
| ATOM | 2681 | NE2 | HIS | 48 | 24.330 | 31.816 | -7.710 | 1.00 | 33.30 |
| ATOM | 2682 | H   | HIS | 48 | 21.159 | 28.462 | -3.362 | 1.00 | 0.00  |
| ATOM | 2683 | HD1 | HIS | 48 | 25.904 | 30.997 | -5.169 | 1.00 | 0.00  |
| ATOM | 2684 | HE2 | HIS | 48 | 24.209 | 32.306 | -8.554 | 1.00 | 0.00  |
| ATOM | 2685 | N   | PRO | 49 | 21.104 | 31.598 | -5.173 | 1.00 | 30.34 |
| ATOM | 2686 | CA  | PRO | 49 | 19.912 | 32.056 | -5.897 | 1.00 | 30.07 |
| ATOM | 2687 | C   | PRO | 49 | 19.492 | 31.326 | -7.187 | 1.00 | 23.56 |
| ATOM | 2688 | O   | PRO | 49 | 18.592 | 31.792 | -7.875 | 1.00 | 31.26 |
| ATOM | 2689 | CB  | PRO | 49 | 20.233 | 33.525 | -6.166 | 1.00 | 29.78 |

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|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 2690 | CG   | PRO | 49 | 21.000 | 33.915 | -4.954  | 1.00 | 29.91 |
| ATOM | 2691 | CD   | PRO | 49 | 21.950 | 32.747 | -4.800  | 1.00 | 31.01 |
| ATOM | 2692 | N    | GLN | 50 | 20.099 | 30.188 | -7.511  | 1.00 | 27.66 |
| ATOM | 2693 | CA   | GLN | 50 | 19.724 | 29.481 | -8.733  | 1.00 | 26.78 |
| ATOM | 2694 | C    | GLN | 50 | 20.006 | 27.979 | -8.707  | 1.00 | 25.56 |
| ATOM | 2695 | O    | GLN | 50 | 19.869 | 27.288 | -9.719  | 1.00 | 26.68 |
| ATOM | 2696 | CB   | GLN | 50 | 20.415 | 30.118 | -9.934  | 1.00 | 28.29 |
| ATOM | 2697 | CG   | GLN | 50 | 19.857 | 29.663 | -11.266 | 1.00 | 31.10 |
| ATOM | 2698 | CD   | GLN | 50 | 20.549 | 30.314 | -12.434 | 1.00 | 32.60 |
| ATOM | 2699 | OE1  | GLN | 50 | 21.479 | 31.106 | -12.258 | 1.00 | 34.73 |
| ATOM | 2700 | NE2  | GLN | 50 | 20.107 | 29.981 | -13.640 | 1.00 | 32.63 |
| ATOM | 2701 | H    | GLN | 50 | 20.762 | 29.768 | -6.949  | 1.00 | 0.00  |
| ATOM | 2702 | HE21 | GLN | 50 | 19.396 | 29.305 | -13.699 | 1.00 | 0.00  |
| ATOM | 2703 | HE22 | GLN | 50 | 20.518 | 30.403 | -14.419 | 1.00 | 0.00  |
| ATOM | 2704 | N    | TRP | 51 | 20.360 | 27.467 | -7.540  | 1.00 | 22.55 |
| ATOM | 2705 | CA   | TRP | 51 | 20.645 | 26.055 | -7.403  | 1.00 | 20.61 |
| ATOM | 2706 | C    | TRP | 51 | 19.932 | 25.533 | -6.187  | 1.00 | 20.60 |
| ATOM | 2707 | O    | TRP | 51 | 19.655 | 26.275 | -5.249  | 1.00 | 21.95 |
| ATOM | 2708 | CB   | TRP | 51 | 22.135 | 25.831 | -7.225  | 1.00 | 20.58 |
| ATOM | 2709 | CG   | TRP | 51 | 22.913 | 26.065 | -8.442  | 1.00 | 21.12 |
| ATOM | 2710 | CD1  | TRP | 51 | 23.459 | 27.243 | -8.853  | 1.00 | 20.74 |
| ATOM | 2711 | CD2  | TRP | 51 | 23.261 | 25.091 | -9.426  | 1.00 | 21.74 |
| ATOM | 2712 | NE1  | TRP | 51 | 24.132 | 27.062 | -10.037 | 1.00 | 22.47 |
| ATOM | 2713 | CE2  | TRP | 51 | 24.026 | 25.748 | -10.411 | 1.00 | 21.72 |
| ATOM | 2714 | CE3  | TRP | 51 | 23.000 | 23.723 | -9.569  | 1.00 | 22.40 |
| ATOM | 2715 | C22  | TRP | 51 | 24.538 | 25.087 | -11.530 | 1.00 | 22.08 |
| ATOM | 2716 | C23  | TRP | 51 | 23.511 | 23.061 | -10.684 | 1.00 | 23.51 |
| ATOM | 2717 | CH2  | TRP | 51 | 24.271 | 23.747 | -11.650 | 1.00 | 22.85 |
| ATOM | 2718 | H    | TRP | 51 | 20.359 | 28.006 | -6.724  | 1.00 | 0.00  |
| ATOM | 2719 | HE1  | TRP | 51 | 24.588 | 27.744 | -10.577 | 1.00 | 0.00  |
| ATOM | 2720 | N    | VAL | 52 | 19.642 | 24.246 | -6.194  | 1.00 | 20.29 |
| ATOM | 2721 | CA   | VAL | 52 | 18.977 | 23.631 | -5.070  | 1.00 | 20.05 |
| ATOM | 2722 | C    | VAL | 52 | 19.770 | 22.384 | -4.722  | 1.00 | 19.26 |
| ATOM | 2723 | O    | VAL | 52 | 20.294 | 21.699 | -5.608  | 1.00 | 18.68 |
| ATOM | 2724 | CB   | VAL | 52 | 17.521 | 23.267 | -5.415  | 1.00 | 21.89 |
| ATOM | 2725 | CG1  | VAL | 52 | 16.800 | 22.733 | -4.185  | 1.00 | 23.63 |
| ATOM | 2726 | CG2  | VAL | 52 | 16.792 | 24.488 | -5.957  | 1.00 | 22.79 |
| ATOM | 2727 | H    | VAL | 52 | 19.849 | 23.708 | -6.986  | 1.00 | 0.00  |
| ATOM | 2728 | N    | LEU | 53 | 19.927 | 22.151 | -3.426  | 1.00 | 18.21 |
| ATOM | 2729 | CA   | LEU | 53 | 20.655 | 20.995 | -2.931  | 1.00 | 17.23 |
| ATOM | 2730 | C    | LEU | 53 | 19.628 | 19.984 | -2.434  | 1.00 | 17.42 |
| ATOM | 2731 | O    | LEU | 53 | 18.676 | 20.343 | -1.735  | 1.00 | 17.68 |
| ATOM | 2732 | CB   | LEU | 53 | 21.604 | 21.423 | -1.807  | 1.00 | 15.02 |
| ATOM | 2733 | CG   | LEU | 53 | 22.556 | 20.410 | -1.177  | 1.00 | 12.62 |
| ATOM | 2734 | CD1  | LEU | 53 | 23.370 | 19.700 | -2.234  | 1.00 | 12.84 |
| ATOM | 2735 | CD2  | LEU | 53 | 23.459 | 21.137 | -0.210  | 1.00 | 12.00 |
| ATOM | 2736 | H    | LEU | 53 | 19.536 | 22.787 | -2.792  | 1.00 | 0.00  |
| ATOM | 2737 | N    | THR | 54 | 19.802 | 18.732 | -2.827  | 1.00 | 17.53 |
| ATOM | 2738 | CA   | THR | 54 | 18.878 | 17.684 | -2.436  | 1.00 | 19.37 |
| ATOM | 2739 | C    | THR | 54 | 19.627 | 16.368 | -2.412  | 1.00 | 20.64 |
| ATOM | 2740 | O    | THR | 54 | 20.732 | 16.270 | -2.949  | 1.00 | 22.18 |
| ATOM | 2741 | CB   | THR | 54 | 17.708 | 17.573 | -3.444  | 1.00 | 19.81 |
| ATOM | 2742 | OG1  | THR | 54 | 16.767 | 16.593 | -2.990  | 1.00 | 20.34 |
| ATOM | 2743 | CG2  | THR | 54 | 18.222 | 17.172 | -4.823  | 1.00 | 18.84 |
| ATOM | 2744 | H    | THR | 54 | 20.562 | 18.501 | -3.407  | 1.00 | 0.00  |
| ATOM | 2745 | HG1  | THR | 54 | 17.052 | 15.713 | -3.244  | 1.00 | 0.00  |
| ATOM | 2746 | N    | ALA | 55 | 19.032 | 15.369 | -1.766  | 1.00 | 20.18 |
| ATOM | 2747 | CA   | ALA | 55 | 19.622 | 14.040 | -1.678  | 1.00 | 19.11 |
| ATOM | 2748 | C    | ALA | 55 | 19.480 | 13.435 | -3.067  | 1.00 | 19.11 |
| ATOM | 2749 | O    | ALA | 55 | 18.418 | 13.518 | -3.684  | 1.00 | 19.41 |
| ATOM | 2750 | CB   | ALA | 55 | 18.881 | 13.191 | -0.645  | 1.00 | 17.89 |
| ATOM | 2751 | H    | ALA | 55 | 18.154 | 15.567 | -1.391  | 1.00 | 0.00  |
| ATOM | 2752 | N    | ALA | 56 | 20.555 | 12.841 | -3.563  | 1.00 | 18.83 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2753 | CA  | ALA | 56  | 20.552 | 12.249 | -4.886  | 1.00 | 17.36 |
| ATOM | 2754 | C   | ALA | 56  | 19.450 | 11.221 | -5.051  | 1.00 | 17.46 |
| ATOM | 2755 | O   | ALA | 56  | 18.778 | 11.198 | -6.076  | 1.00 | 18.33 |
| ATOM | 2756 | CB  | ALA | 56  | 21.892 | 11.624 | -5.179  | 1.00 | 16.53 |
| ATOM | 2757 | H   | ALA | 56  | 21.351 | 12.744 | -2.995  | 1.00 | 0.00  |
| ATOM | 2758 | N   | HIS | 57  | 19.200 | 10.424 | -4.019  | 1.00 | 17.19 |
| ATOM | 2759 | CA  | HIS | 57  | 18.180 | 9.388  | -4.135  | 1.00 | 17.54 |
| ATOM | 2760 | C   | HIS | 57  | 16.794 | 9.884  | -4.509  | 1.00 | 17.73 |
| ATOM | 2761 | O   | HIS | 57  | 15.974 | 9.104  | -5.003  | 1.00 | 19.07 |
| ATOM | 2762 | CB  | HIS | 57  | 18.140 | 8.458  | -2.912  | 1.00 | 15.19 |
| ATOM | 2763 | CG  | HIS | 57  | 17.451 | 9.028  | -1.716  | 1.00 | 13.02 |
| ATOM | 2764 | ND1 | HIS | 57  | 18.109 | 9.781  | -0.770  | 1.00 | 14.48 |
| ATOM | 2765 | CD2 | HIS | 57  | 16.182 | 8.885  | -1.266  | 1.00 | 12.46 |
| ATOM | 2766 | CE1 | HIS | 57  | 17.280 | 10.071 | 0.217   | 1.00 | 14.99 |
| ATOM | 2767 | NE2 | HIS | 57  | 16.104 | 9.540  | -0.060  | 1.00 | 13.56 |
| ATOM | 2768 | H   | HIS | 57  | 19.735 | 10.539 | -3.222  | 1.00 | 0.00  |
| ATOM | 2769 | HD1 | HIS | 57  | 19.029 | 10.101 | -0.797  | 1.00 | 0.00  |
| ATOM | 2770 | HE2 | HIS | 57  | 15.364 | 9.660  | 0.589   | 1.00 | 0.00  |
| ATOM | 2771 | N   | CYS | 58  | 16.557 | 11.183 | -4.325  | 1.00 | 15.90 |
| ATOM | 2772 | CA  | CYS | 58  | 15.270 | 11.781 | -4.664  | 1.00 | 13.65 |
| ATOM | 2773 | C   | CYS | 58  | 15.140 | 11.922 | -6.171  | 1.00 | 13.01 |
| ATOM | 2774 | O   | CYS | 58  | 14.041 | 11.869 | -6.716  | 1.00 | 12.43 |
| ATOM | 2775 | CB  | CYS | 58  | 15.115 | 13.157 | -4.011  | 1.00 | 11.81 |
| ATOM | 2776 | SG  | CYS | 58  | 14.878 | 13.143 | -2.206  | 1.00 | 12.16 |
| ATOM | 2777 | H   | CYS | 58  | 17.254 | 11.786 | -4.000  | 1.00 | 0.00  |
| ATOM | 2778 | N   | VAL | 59  | 16.269 | 12.060 | -6.850  | 1.00 | 13.50 |
| ATOM | 2779 | CA  | VAL | 59  | 16.254 | 12.235 | -8.287  | 1.00 | 15.24 |
| ATOM | 2780 | C   | VAL | 59  | 17.119 | 11.230 | -9.051  | 1.00 | 16.81 |
| ATOM | 2781 | O   | VAL | 59  | 17.322 | 11.381 | -10.255 | 1.00 | 17.91 |
| ATOM | 2782 | CB  | VAL | 59  | 16.652 | 13.692 | -8.653  | 1.00 | 15.93 |
| ATOM | 2783 | CG1 | VAL | 59  | 15.678 | 14.675 | -8.019  | 1.00 | 15.10 |
| ATOM | 2784 | CG2 | VAL | 59  | 18.055 | 14.000 | -8.162  | 1.00 | 16.07 |
| ATOM | 2785 | H   | VAL | 59  | 17.135 | 12.040 | -6.403  | 1.00 | 0.00  |
| ATOM | 2786 | N   | GLY | 60  | 17.565 | 10.171 | -8.377  | 1.00 | 18.29 |
| ATOM | 2787 | CA  | GLY | 60  | 18.400 | 9.171  | -9.027  | 1.00 | 19.78 |
| ATOM | 2788 | C   | GLY | 60  | 18.211 | 7.780  | -8.448  | 1.00 | 21.73 |
| ATOM | 2789 | O   | GLY | 60  | 17.307 | 7.587  | -7.633  | 1.00 | 22.76 |
| ATOM | 2790 | H   | GLY | 60  | 17.367 | 10.069 | -7.421  | 1.00 | 0.00  |
| ATOM | 2791 | N   | PRO | 60A | 19.035 | 6.786  | -8.836  | 1.00 | 22.38 |
| ATOM | 2792 | CA  | PRO | 60A | 20.102 | 6.848  | -9.840  | 1.00 | 23.99 |
| ATOM | 2793 | C   | PRO | 60A | 19.603 | 6.798  | -11.284 | 1.00 | 26.78 |
| ATOM | 2794 | O   | PRO | 60A | 20.330 | 7.160  | -12.211 | 1.00 | 26.72 |
| ATOM | 2795 | CB  | PRO | 60A | 20.949 | 5.627  | -9.499  | 1.00 | 22.26 |
| ATOM | 2796 | CG  | PRO | 60A | 19.927 | 4.652  | -9.071  | 1.00 | 21.97 |
| ATOM | 2797 | CD  | PRO | 60A | 19.061 | 5.483  | -8.153  | 1.00 | 21.93 |
| ATOM | 2798 | N   | ASP | 60B | 18.385 | 6.312  | -11.483 | 1.00 | 29.92 |
| ATOM | 2799 | CA  | ASP | 60B | 17.815 | 6.248  | -12.821 | 1.00 | 32.24 |
| ATOM | 2800 | C   | ASP | 60B | 17.413 | 7.643  | -13.261 | 1.00 | 32.61 |
| ATOM | 2801 | O   | ASP | 60B | 16.755 | 8.369  | -12.508 | 1.00 | 33.74 |
| ATOM | 2802 | CB  | ASP | 60B | 16.625 | 5.295  | -12.852 | 1.00 | 35.70 |
| ATOM | 2803 | CG  | ASP | 60B | 17.052 | 3.843  | -13.013 | 1.00 | 39.63 |
| ATOM | 2804 | OD1 | ASP | 60B | 16.328 | 3.088  | -13.698 | 1.00 | 42.71 |
| ATOM | 2805 | OD2 | ASP | 60B | 18.124 | 3.463  | -12.486 | 1.00 | 39.48 |
| ATOM | 2806 | H   | ASP | 60B | 17.877 | 5.898  | -10.759 | 1.00 | 0.00  |
| ATOM | 2807 | N   | VAL | 60C | 17.825 | 8.010  | -14.471 | 1.00 | 32.19 |
| ATOM | 2808 | CA  | VAL | 60C | 17.566 | 9.328  | -15.042 | 1.00 | 31.81 |
| ATOM | 2809 | C   | VAL | 60C | 16.098 | 9.726  | -15.061 | 1.00 | 32.78 |
| ATOM | 2810 | O   | VAL | 60C | 15.241 | 8.972  | -15.521 | 1.00 | 31.88 |
| ATOM | 2811 | CB  | VAL | 60C | 18.128 | 9.439  | -16.465 | 1.00 | 30.90 |
| ATOM | 2812 | CG1 | VAL | 60C | 17.951 | 10.853 | -16.988 | 1.00 | 31.50 |
| ATOM | 2813 | CG2 | VAL | 60C | 19.585 | 9.053  | -16.480 | 1.00 | 30.47 |
| ATOM | 2814 | H   | VAL | 60C | 18.260 | 7.321  | -14.992 | 1.00 | 0.00  |
| ATOM | 2815 | N   | LYS | 60D | 15.827 | 10.931 | -14.571 | 1.00 | 34.63 |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2816 | CA  | LYS | 60D | 14.473 | 11.471 | -14.516 | 1.00 | 36.61 |
| ATOM | 2817 | C   | LYS | 60D | 14.276 | 12.493 | -15.639 | 1.00 | 37.86 |
| ATOM | 2818 | O   | LYS | 60D | 15.255 | 12.944 | -16.248 | 1.00 | 38.80 |
| ATOM | 2819 | CB  | LYS | 60D | 14.231 | 12.134 | -13.156 | 1.00 | 37.46 |
| ATOM | 2820 | CG  | LYS | 60D | 14.432 | 11.209 | -11.958 | 1.00 | 39.46 |
| ATOM | 2821 | CD  | LYS | 60D | 13.524 | 9.976  | -12.021 | 1.00 | 41.12 |
| ATOM | 2822 | CE  | LYS | 60D | 13.587 | 9.147  | -10.743 | 1.00 | 41.39 |
| ATOM | 2823 | NZ  | LYS | 60D | 14.981 | 8.765  | -10.396 | 1.00 | 42.83 |
| ATOM | 2824 | H   | LYS | 60D | 16.579 | 11.494 | -14.309 | 1.00 | 0.00  |
| ATOM | 2825 | HZ1 | LYS | 60D | 15.530 | 9.628  | -10.211 | 1.00 | 0.00  |
| ATOM | 2826 | HZ2 | LYS | 60D | 15.444 | 8.311  | -11.221 | 1.00 | 0.00  |
| ATOM | 2827 | HZ3 | LYS | 60D | 15.003 | 8.161  | -9.553  | 1.00 | 0.00  |
| ATOM | 2828 | N   | ASP | 60E | 13.018 | 12.835 | -15.927 | 1.00 | 37.69 |
| ATOM | 2829 | CA  | ASP | 60E | 12.687 | 13.813 | -16.971 | 1.00 | 36.59 |
| ATOM | 2830 | C   | ASP | 60E | 12.401 | 15.168 | -16.319 | 1.00 | 34.20 |
| ATOM | 2831 | O   | ASP | 60E | 11.424 | 15.321 | -15.585 | 1.00 | 35.05 |
| ATOM | 2832 | CB  | ASP | 60E | 11.468 | 13.344 | -17.780 | 1.00 | 39.68 |
| ATOM | 2833 | CG  | ASP | 60E | 11.082 | 14.316 | -18.901 | 1.00 | 42.67 |
| ATOM | 2834 | OD1 | ASP | 60E | 11.798 | 15.318 | -19.148 | 1.00 | 43.63 |
| ATOM | 2835 | OD2 | ASP | 60E | 10.042 | 14.073 | -19.551 | 1.00 | 44.07 |
| ATOM | 2836 | H   | ASP | 60E | 12.267 | 12.460 | -15.423 | 1.00 | 0.00  |
| ATOM | 2837 | N   | LEU | 61  | 13.233 | 16.157 | -16.628 | 1.00 | 30.70 |
| ATOM | 2838 | CA  | LEU | 61  | 13.104 | 17.495 | -16.058 | 1.00 | 28.24 |
| ATOM | 2839 | C   | LEU | 61  | 11.737 | 18.127 | -16.259 | 1.00 | 27.08 |
| ATOM | 2840 | O   | LEU | 61  | 11.274 | 18.901 | -15.415 | 1.00 | 26.94 |
| ATOM | 2841 | CB  | LEU | 61  | 14.184 | 18.420 | -16.614 | 1.00 | 28.43 |
| ATOM | 2842 | CG  | LEU | 61  | 15.621 | 18.307 | -16.103 | 1.00 | 27.91 |
| ATOM | 2843 | CD1 | LEU | 61  | 16.104 | 16.877 | -16.139 | 1.00 | 28.27 |
| ATOM | 2844 | CD2 | LEU | 61  | 16.511 | 19.182 | -16.968 | 1.00 | 29.59 |
| ATOM | 2845 | H   | LEU | 61  | 13.920 | 15.959 | -17.295 | 1.00 | 0.00  |
| ATOM | 2846 | N   | ALA | 62  | 11.082 | 17.784 | -17.364 | 1.00 | 26.52 |
| ATOM | 2847 | CA  | ALA | 62  | 9.757  | 18.320 | -17.664 | 1.00 | 25.24 |
| ATOM | 2848 | C   | ALA | 62  | 8.742  | 17.859 | -16.616 | 1.00 | 24.34 |
| ATOM | 2849 | O   | ALA | 62  | 7.679  | 18.462 | -16.459 | 1.00 | 24.36 |
| ATOM | 2850 | CB  | ALA | 62  | 9.313  | 17.884 | -19.056 | 1.00 | 23.95 |
| ATOM | 2851 | H   | ALA | 62  | 11.490 | 17.124 | -17.969 | 1.00 | 0.00  |
| ATOM | 2852 | N   | ALA | 63  | 9.076  | 16.779 | -15.917 | 1.00 | 23.30 |
| ATOM | 2853 | CA  | ALA | 63  | 8.213  | 16.212 | -14.891 | 1.00 | 23.20 |
| ATOM | 2854 | C   | ALA | 63  | 8.484  | 16.808 | -13.514 | 1.00 | 22.80 |
| ATOM | 2855 | O   | ALA | 63  | 7.712  | 16.593 | -12.577 | 1.00 | 22.80 |
| ATOM | 2856 | CB  | ALA | 63  | 8.386  | 14.698 | -14.851 | 1.00 | 22.57 |
| ATOM | 2857 | H   | ALA | 63  | 9.919  | 16.312 | -16.072 | 1.00 | 0.00  |
| ATOM | 2858 | N   | LEU | 64  | 9.569  | 17.565 | -13.403 | 1.00 | 22.39 |
| ATOM | 2859 | CA  | LEU | 64  | 9.953  | 18.176 | -12.143 | 1.00 | 23.25 |
| ATOM | 2860 | C   | LEU | 64  | 9.691  | 19.673 | -12.040 | 1.00 | 23.93 |
| ATOM | 2861 | O   | LEU | 64  | 9.748  | 20.421 | -13.029 | 1.00 | 24.43 |
| ATOM | 2862 | CB  | LEU | 64  | 11.432 | 17.929 | -11.854 | 1.00 | 24.96 |
| ATOM | 2863 | CG  | LEU | 64  | 11.853 | 16.614 | -11.213 | 1.00 | 26.97 |
| ATOM | 2864 | CD1 | LEU | 64  | 11.580 | 15.442 | -12.152 | 1.00 | 28.52 |
| ATOM | 2865 | CD2 | LEU | 64  | 13.329 | 16.705 | -10.882 | 1.00 | 26.77 |
| ATOM | 2866 | H   | LEU | 64  | 10.108 | 17.782 | -14.188 | 1.00 | 0.00  |
| ATOM | 2867 | N   | ARG | 65  | 9.471  | 20.104 | -10.805 | 1.00 | 23.23 |
| ATOM | 2868 | CA  | ARG | 65  | 9.219  | 21.493 | -10.474 | 1.00 | 22.50 |
| ATOM | 2869 | C   | ARG | 65  | 9.721  | 21.704 | -9.052  | 1.00 | 22.11 |
| ATOM | 2870 | O   | ARG | 65  | 9.804  | 20.750 | -8.271  | 1.00 | 22.73 |
| ATOM | 2871 | CB  | ARG | 65  | 7.721  | 21.796 | -10.531 | 1.00 | 23.16 |
| ATOM | 2872 | CG  | ARG | 65  | 7.140  | 21.829 | -11.914 | 1.00 | 22.86 |
| ATOM | 2873 | CD  | ARG | 65  | 7.728  | 22.963 | -12.699 | 1.00 | 25.08 |
| ATOM | 2874 | NE  | ARG | 65  | 7.825  | 22.594 | -14.100 | 1.00 | 27.11 |
| ATOM | 2875 | CZ  | ARG | 65  | 6.877  | 22.819 | -14.999 | 1.00 | 27.62 |
| ATOM | 2876 | NH1 | ARG | 65  | 5.749  | 23.428 | -14.643 | 1.00 | 28.46 |
| ATOM | 2877 | NH2 | ARG | 65  | 7.047  | 22.393 | -16.241 | 1.00 | 28.68 |
| ATOM | 2878 | H   | ARG | 65  | 9.476  | 19.442 | -10.080 | 1.00 | 0.00  |

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|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 2879 | HE   | ARG | 65 | 8.651  | 22.085 | -14.311 | 1.00 | 0.00  |
| ATOM | 2880 | HH11 | ARG | 65 | 5.617  | 23.715 | -13.689 | 1.00 | 0.00  |
| ATOM | 2881 | HH12 | ARG | 65 | 5.006  | 23.621 | -15.284 | 1.00 | 0.00  |
| ATOM | 2882 | HH21 | ARG | 65 | 7.879  | 21.881 | -16.479 | 1.00 | 0.00  |
| ATOM | 2883 | HH22 | ARG | 65 | 6.370  | 22.515 | -16.970 | 1.00 | 0.00  |
| ATOM | 2884 | N    | VAL | 66 | 10.043 | 22.953 | -8.728  | 1.00 | 20.10 |
| ATOM | 2885 | CA   | VAL | 66 | 10.530 | 23.338 | -7.409  | 1.00 | 17.28 |
| ATOM | 2886 | C    | VAL | 66 | 9.613  | 24.402 | -6.799  | 1.00 | 17.58 |
| ATOM | 2887 | O    | VAL | 66 | 9.236  | 25.367 | -7.466  | 1.00 | 18.98 |
| ATOM | 2888 | CB   | VAL | 66 | 11.956 | 23.919 | -7.511  | 1.00 | 14.84 |
| ATOM | 2889 | CG1  | VAL | 66 | 12.364 | 24.570 | -6.205  | 1.00 | 14.99 |
| ATOM | 2890 | CG2  | VAL | 66 | 12.933 | 22.825 | -7.878  | 1.00 | 14.12 |
| ATOM | 2891 | H    | VAL | 66 | 9.993  | 23.638 | -9.420  | 1.00 | 0.00  |
| ATOM | 2892 | N    | GLN | 67 | 9.212  | 24.196 | -5.555  | 1.00 | 15.80 |
| ATOM | 2893 | CA   | GLN | 67 | 8.375  | 25.158 | -4.858  | 1.00 | 14.72 |
| ATOM | 2894 | C    | GLN | 67 | 9.218  | 25.660 | -3.724  | 1.00 | 14.29 |
| ATOM | 2895 | O    | GLN | 67 | 9.722  | 24.868 | -2.950  | 1.00 | 16.53 |
| ATOM | 2896 | CB   | GLN | 67 | 7.131  | 24.485 | -4.291  | 1.00 | 14.76 |
| ATOM | 2897 | CG   | GLN | 67 | 6.405  | 25.311 | -3.242  | 1.00 | 16.40 |
| ATOM | 2898 | CD   | GLN | 67 | 5.834  | 26.622 | -3.776  | 1.00 | 19.05 |
| ATOM | 2899 | OE1  | GLN | 67 | 6.067  | 27.011 | -4.924  | 1.00 | 19.16 |
| ATOM | 2900 | NE2  | GLN | 67 | 5.085  | 27.313 | -2.934  | 1.00 | 20.50 |
| ATOM | 2901 | H    | GLN | 67 | 9.454  | 23.368 | -5.096  | 1.00 | 0.00  |
| ATOM | 2902 | HE21 | GLN | 67 | 5.053  | 26.945 | -2.028  | 1.00 | 0.00  |
| ATOM | 2903 | HE22 | GLN | 67 | 4.519  | 28.065 | -3.191  | 1.00 | 0.00  |
| ATOM | 2904 | N    | LEU | 68 | 9.380  | 26.965 | -3.615  | 1.00 | 15.17 |
| ATOM | 2905 | CA   | LEU | 68 | 10.193 | 27.518 | -2.537  | 1.00 | 18.04 |
| ATOM | 2906 | C    | LEU | 68 | 9.415  | 27.477 | -1.221  | 1.00 | 19.10 |
| ATOM | 2907 | O    | LEU | 68 | 8.333  | 26.897 | -1.169  | 1.00 | 20.36 |
| ATOM | 2908 | CB   | LEU | 68 | 10.632 | 28.945 | -2.889  | 1.00 | 19.50 |
| ATOM | 2909 | CG   | LEU | 68 | 11.272 | 29.107 | -4.282  | 1.00 | 21.10 |
| ATOM | 2910 | CD1  | LEU | 68 | 11.599 | 30.560 | -4.562  | 1.00 | 21.08 |
| ATOM | 2911 | CD2  | LEU | 68 | 12.521 | 28.239 | -4.414  | 1.00 | 21.93 |
| ATOM | 2912 | H    | LEU | 68 | 8.938  | 27.552 | -4.261  | 1.00 | 0.00  |
| ATOM | 2913 | N    | ARG | 69 | 9.985  | 28.052 | -0.162  | 1.00 | 20.44 |
| ATOM | 2914 | CA   | ARG | 69 | 9.364  | 28.095 | 1.173   | 1.00 | 21.26 |
| ATOM | 2915 | C    | ARG | 69 | 7.858  | 28.324 | 1.116   | 1.00 | 21.99 |
| ATOM | 2916 | O    | ARG | 69 | 7.398  | 29.319 | 0.559   | 1.00 | 23.44 |
| ATOM | 2917 | CB   | ARG | 69 | 10.009 | 29.204 | 2.007   | 1.00 | 22.01 |
| ATOM | 2918 | CG   | ARG | 69 | 9.411  | 29.425 | 3.395   | 1.00 | 21.35 |
| ATOM | 2919 | CD   | ARG | 69 | 9.821  | 28.351 | 4.375   | 1.00 | 19.91 |
| ATOM | 2920 | NE   | ARG | 69 | 9.553  | 28.744 | 5.757   | 1.00 | 20.69 |
| ATOM | 2921 | CZ   | ARG | 69 | 8.345  | 28.740 | 6.320   | 1.00 | 20.75 |
| ATOM | 2922 | NH1  | ARG | 69 | 7.282  | 28.373 | 5.620   | 1.00 | 20.48 |
| ATOM | 2923 | NH2  | ARG | 69 | 8.196  | 29.057 | 7.598   | 1.00 | 20.48 |
| ATOM | 2924 | H    | ARG | 69 | 10.883 | 28.425 | -0.269  | 1.00 | 0.00  |
| ATOM | 2925 | HE   | ARG | 69 | 10.338 | 29.042 | 6.252   | 1.00 | 0.00  |
| ATOM | 2926 | HH11 | ARG | 69 | 7.358  | 28.083 | 4.667   | 1.00 | 0.00  |
| ATOM | 2927 | HH12 | ARG | 69 | 6.391  | 28.356 | 6.084   | 1.00 | 0.00  |
| ATOM | 2928 | HH21 | ARG | 69 | 8.889  | 29.324 | 8.257   | 1.00 | 0.00  |
| ATOM | 2929 | HH22 | ARG | 69 | 7.266  | 29.001 | 7.985   | 1.00 | 0.00  |
| ATOM | 2930 | N    | GLU | 70 | 7.103  | 27.445 | 1.764   | 1.00 | 21.84 |
| ATOM | 2931 | CA   | GLU | 70 | 5.651  | 27.532 | 1.763   | 1.00 | 22.23 |
| ATOM | 2932 | C    | GLU | 70 | 5.104  | 26.969 | 3.076   | 1.00 | 23.30 |
| ATOM | 2933 | O    | GLU | 70 | 5.443  | 25.846 | 3.452   | 1.00 | 23.20 |
| ATOM | 2934 | CB   | GLU | 70 | 5.139  | 26.719 | 0.576   | 1.00 | 21.53 |
| ATOM | 2935 | CG   | GLU | 70 | 3.662  | 26.816 | 0.277   | 1.00 | 21.77 |
| ATOM | 2936 | CD   | GLU | 70 | 3.311  | 26.073 | -0.996  | 1.00 | 22.44 |
| ATOM | 2937 | OE1  | GLU | 70 | 2.392  | 26.511 | -1.718  | 1.00 | 23.02 |
| ATOM | 2938 | OE2  | GLU | 70 | 3.987  | 25.065 | -1.297  | 1.00 | 22.45 |
| ATOM | 2939 | H    | GLU | 70 | 7.514  | 26.683 | 2.224   | 1.00 | 0.00  |
| ATOM | 2940 | N    | GLN | 71 | 4.300  | 27.754 | 3.795   | 1.00 | 24.46 |
| ATOM | 2941 | CA   | GLN | 71 | 3.733  | 27.296 | 5.073   | 1.00 | 26.04 |

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|------|------|------|-----|----|--------|--------|--------|------|-------|
| ATOM | 2942 | C    | GLN | 71 | 2.814  | 26.089 | 4.968  | 1.00 | 27.48 |
| ATOM | 2943 | O    | GLN | 71 | 2.712  | 25.314 | 5.923  | 1.00 | 29.36 |
| ATOM | 2944 | CB   | GLN | 71 | 2.951  | 28.402 | 5.779  | 1.00 | 26.68 |
| ATOM | 2945 | CG   | GLN | 71 | 3.752  | 29.246 | 6.749  | 1.00 | 28.96 |
| ATOM | 2946 | CD   | GLN | 71 | 4.430  | 28.450 | 7.855  | 1.00 | 28.60 |
| ATOM | 2947 | OE1  | GLN | 71 | 5.638  | 28.574 | 8.048  | 1.00 | 30.20 |
| ATOM | 2948 | NE2  | GLN | 71 | 3.665  | 27.659 | 8.595  | 1.00 | 27.33 |
| ATOM | 2949 | H    | GLN | 71 | 4.068  | 28.640 | 3.448  | 1.00 | 0.00  |
| ATOM | 2950 | HE21 | GLN | 71 | 2.713  | 27.548 | 8.437  | 1.00 | 0.00  |
| ATOM | 2951 | HE22 | GLN | 71 | 4.140  | 27.223 | 9.342  | 1.00 | 0.00  |
| ATOM | 2952 | N    | HIS | 72 | 2.100  | 25.967 | 3.850  | 1.00 | 26.56 |
| ATOM | 2953 | CA   | HIS | 72 | 1.176  | 24.860 | 3.651  | 1.00 | 25.54 |
| ATOM | 2954 | C    | HIS | 72 | 1.350  | 24.268 | 2.259  | 1.00 | 26.53 |
| ATOM | 2955 | O    | HIS | 72 | 1.008  | 24.893 | 1.254  | 1.00 | 26.89 |
| ATOM | 2956 | CB   | HIS | 72 | -0.246 | 25.337 | 3.905  | 1.00 | 24.25 |
| ATOM | 2957 | CG   | HIS | 72 | -0.465 | 25.802 | 5.309  | 1.00 | 24.96 |
| ATOM | 2958 | ND1  | HIS | 72 | -0.510 | 24.935 | 6.379  | 1.00 | 25.83 |
| ATOM | 2959 | CD2  | HIS | 72 | -0.607 | 27.045 | 5.829  | 1.00 | 24.79 |
| ATOM | 2960 | CE1  | HIS | 72 | -0.671 | 25.619 | 7.497  | 1.00 | 25.14 |
| ATOM | 2961 | NE2  | HIS | 72 | -0.733 | 26.902 | 7.190  | 1.00 | 24.96 |
| ATOM | 2962 | H    | HIS | 72 | 2.210  | 26.584 | 3.096  | 1.00 | 0.00  |
| ATOM | 2963 | HD1  | HIS | 72 | -0.410 | 23.963 | 6.263  | 1.00 | 0.00  |
| ATOM | 2964 | HE2  | HIS | 72 | -0.864 | 27.615 | 7.848  | 1.00 | 0.00  |
| ATOM | 2965 | N    | LEU | 73 | 1.809  | 23.018 | 2.242  | 1.00 | 26.03 |
| ATOM | 2966 | CA   | LEU | 73 | 2.134  | 22.267 | 1.030  | 1.00 | 26.58 |
| ATOM | 2967 | C    | LEU | 73 | 1.599  | 22.527 | -0.360 | 1.00 | 27.02 |
| ATOM | 2968 | O    | LEU | 73 | 2.320  | 22.252 | -1.321 | 1.00 | 30.14 |
| ATOM | 2969 | CB   | LEU | 73 | 2.090  | 20.760 | 1.266  | 1.00 | 26.60 |
| ATOM | 2970 | CG   | LEU | 73 | 3.444  | 20.068 | 1.433  | 1.00 | 25.39 |
| ATOM | 2971 | CD1  | LEU | 73 | 3.340  | 18.656 | 0.913  | 1.00 | 25.50 |
| ATOM | 2972 | CD2  | LEU | 73 | 4.535  | 20.811 | 0.687  | 1.00 | 25.01 |
| ATOM | 2973 | H    | LEU | 73 | 1.958  | 22.584 | 3.113  | 1.00 | 0.00  |
| ATOM | 2974 | N    | TYR | 74 | 0.343  | 22.917 | -0.519 | 1.00 | 24.10 |
| ATOM | 2975 | CA   | TYR | 74 | -0.130 | 23.149 | -1.879 | 1.00 | 23.81 |
| ATOM | 2976 | C    | TYR | 74 | -0.955 | 24.408 | -1.978 | 1.00 | 27.06 |
| ATOM | 2977 | O    | TYR | 74 | -1.572 | 24.693 | -3.003 | 1.00 | 26.99 |
| ATOM | 2978 | CB   | TYR | 74 | -0.928 | 21.950 | -2.373 | 1.00 | 20.11 |
| ATOM | 2979 | CG   | TYR | 74 | -0.182 | 20.644 | -2.260 | 1.00 | 17.05 |
| ATOM | 2980 | CD1  | TYR | 74 | -0.371 | 19.809 | -1.162 | 1.00 | 16.55 |
| ATOM | 2981 | CD2  | TYR | 74 | 0.718  | 20.246 | -3.242 | 1.00 | 15.21 |
| ATOM | 2982 | CE1  | TYR | 74 | 0.319  | 18.611 | -1.044 | 1.00 | 15.49 |
| ATOM | 2983 | CE2  | TYR | 74 | 1.411  | 19.053 | -3.134 | 1.00 | 14.58 |
| ATOM | 2984 | CZ   | TYR | 74 | 1.208  | 18.238 | -2.036 | 1.00 | 15.33 |
| ATOM | 2985 | OH   | TYR | 74 | 1.889  | 17.047 | -1.926 | 1.00 | 16.08 |
| ATOM | 2986 | H    | TYR | 74 | -0.229 | 23.081 | 0.248  | 1.00 | 0.00  |
| ATOM | 2987 | HH   | TYR | 74 | 1.801  | 16.700 | -1.028 | 1.00 | 0.00  |
| ATOM | 2988 | N    | TYR | 75 | -0.931 | 25.186 | -0.910 | 1.00 | 31.65 |
| ATOM | 2989 | CA   | TYR | 75 | -1.701 | 26.404 | -0.846 | 1.00 | 36.39 |
| ATOM | 2990 | C    | TYR | 75 | -0.778 | 27.556 | -1.244 | 1.00 | 39.17 |
| ATOM | 2991 | O    | TYR | 75 | 0.125  | 27.939 | -0.495 | 1.00 | 41.04 |
| ATOM | 2992 | CB   | TYR | 75 | -2.295 | 26.557 | 0.568  | 1.00 | 39.44 |
| ATOM | 2993 | CG   | TYR | 75 | -3.060 | 25.311 | 1.049  | 1.00 | 42.68 |
| ATOM | 2994 | CD1  | TYR | 75 | -2.380 | 24.169 | 1.493  | 1.00 | 44.08 |
| ATOM | 2995 | CD2  | TYR | 75 | -4.455 | 25.262 | 1.028  | 1.00 | 43.19 |
| ATOM | 2996 | CE1  | TYR | 75 | -3.073 | 23.015 | 1.898  | 1.00 | 43.78 |
| ATOM | 2997 | CE2  | TYR | 75 | -5.153 | 24.109 | 1.433  | 1.00 | 43.52 |
| ATOM | 2998 | CZ   | TYR | 75 | -4.455 | 22.994 | 1.866  | 1.00 | 43.62 |
| ATOM | 2999 | OH   | TYR | 75 | -5.137 | 21.864 | 2.268  | 1.00 | 43.43 |
| ATOM | 3000 | H    | TYR | 75 | -0.265 | 25.020 | -0.212 | 1.00 | 0.00  |
| ATOM | 3001 | HH   | TYR | 75 | -6.095 | 22.027 | 2.259  | 1.00 | 0.00  |
| ATOM | 3002 | N    | GLN | 79 | -1.011 | 28.062 | -2.454 | 1.00 | 40.20 |
| ATOM | 3003 | CA   | GLN | 79 | -0.256 | 29.155 | -3.079 | 1.00 | 40.33 |
| ATOM | 3004 | C    | GLN | 79 | 0.962  | 28.596 | -3.789 | 1.00 | 37.64 |

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|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 3005 | O    | GLN | 79 | 2.074  | 29.115 | -3.683  | 1.00 | 36.67 |
| ATOM | 3006 | CB   | GLN | 79 | 0.124  | 30.271 | -2.086  | 1.00 | 45.26 |
| ATOM | 3007 | CG   | GLN | 79 | 0.853  | 31.509 | -2.704  | 1.00 | 51.67 |
| ATOM | 3008 | CD   | GLN | 79 | 0.066  | 32.239 | -3.813  | 1.00 | 54.23 |
| ATOM | 3009 | OE1  | GLN | 79 | -1.125 | 32.540 | -3.664  | 1.00 | 55.60 |
| ATOM | 3010 | NE2  | GLN | 79 | 0.750  | 32.553 | -4.913  | 1.00 | 53.74 |
| ATOM | 3011 | H    | GLN | 79 | -1.717 | 27.635 | -2.978  | 1.00 | 0.00  |
| ATOM | 3012 | HE21 | GLN | 79 | 1.706  | 32.319 | -4.951  | 1.00 | 0.00  |
| ATOM | 3013 | HE22 | GLN | 79 | 0.269  | 33.003 | -5.631  | 1.00 | 0.00  |
| ATOM | 3014 | N    | ASP | 80 | 0.730  | 27.512 | -4.514  | 1.00 | 35.38 |
| ATOM | 3015 | CA   | ASP | 80 | 1.781  | 26.876 | -5.280  | 1.00 | 33.84 |
| ATOM | 3016 | C    | ASP | 80 | 2.280  | 27.868 | -6.316  | 1.00 | 33.21 |
| ATOM | 3017 | O    | ASP | 80 | 1.506  | 28.658 | -6.853  | 1.00 | 33.16 |
| ATOM | 3018 | CB   | ASP | 80 | 1.236  | 25.644 | -6.000  | 1.00 | 33.14 |
| ATOM | 3019 | CG   | ASP | 80 | 1.616  | 24.352 | -5.318  | 1.00 | 31.13 |
| ATOM | 3020 | OD1  | ASP | 80 | 2.074  | 24.394 | -4.160  | 1.00 | 30.14 |
| ATOM | 3021 | OD2  | ASP | 80 | 1.468  | 23.286 | -5.952  | 1.00 | 29.87 |
| ATOM | 3022 | H    | ASP | 80 | -0.147 | 27.096 | -4.508  | 1.00 | 0.00  |
| ATOM | 3023 | N    | GLN | 81 | 3.575  | 27.812 | -6.592  | 1.00 | 33.02 |
| ATOM | 3024 | CA   | GLN | 81 | 4.220  | 28.675 | -7.572  | 1.00 | 32.15 |
| ATOM | 3025 | C    | GLN | 81 | 5.454  | 27.907 | -8.035  | 1.00 | 29.69 |
| ATOM | 3026 | O    | GLN | 81 | 6.595  | 28.306 | -7.801  | 1.00 | 29.42 |
| ATOM | 3027 | CB   | GLN | 81 | 4.586  | 30.018 | -6.935  | 1.00 | 35.77 |
| ATOM | 3028 | CG   | GLN | 81 | 5.297  | 29.901 | -5.590  | 1.00 | 41.85 |
| ATOM | 3029 | CD   | GLN | 81 | 4.686  | 30.786 | -4.505  | 1.00 | 45.18 |
| ATOM | 3030 | OE1  | GLN | 81 | 4.149  | 31.867 | -4.783  | 1.00 | 45.71 |
| ATOM | 3031 | NE2  | GLN | 81 | 4.769  | 30.326 | -3.257  | 1.00 | 45.70 |
| ATOM | 3032 | H    | GLN | 81 | 4.122  | 27.157 | -6.102  | 1.00 | 0.00  |
| ATOM | 3033 | HE21 | GLN | 81 | 5.209  | 29.474 | -3.068  | 1.00 | 0.00  |
| ATOM | 3034 | HE22 | GLN | 81 | 4.349  | 30.887 | -2.576  | 1.00 | 0.00  |
| ATOM | 3035 | N    | LEU | 82 | 5.192  | 26.765 | -8.661  | 1.00 | 26.81 |
| ATOM | 3036 | CA   | LEU | 82 | 6.225  | 25.864 | -9.158  | 1.00 | 24.87 |
| ATOM | 3037 | C    | LEU | 82 | 7.261  | 26.524 | -10.070 | 1.00 | 24.59 |
| ATOM | 3038 | O    | LEU | 82 | 6.938  | 27.426 | -10.837 | 1.00 | 26.38 |
| ATOM | 3039 | CB   | LEU | 82 | 5.579  | 24.674 | -9.881  | 1.00 | 21.39 |
| ATOM | 3040 | CG   | LEU | 82 | 4.519  | 23.854 | -9.139  | 1.00 | 18.22 |
| ATOM | 3041 | CD1  | LEU | 82 | 4.728  | 23.958 | -7.647  | 1.00 | 18.78 |
| ATOM | 3042 | CD2  | LEU | 82 | 3.134  | 24.336 | -9.488  | 1.00 | 20.24 |
| ATOM | 3043 | H    | LEU | 82 | 4.250  | 26.550 | -8.792  | 1.00 | 0.00  |
| ATOM | 3044 | N    | LEU | 83 | 8.504  | 26.067 | -9.981  | 1.00 | 22.76 |
| ATOM | 3045 | CA   | LEU | 83 | 9.577  | 26.605 | -10.799 | 1.00 | 22.62 |
| ATOM | 3046 | C    | LEU | 83 | 10.222 | 25.495 | -11.621 | 1.00 | 24.07 |
| ATOM | 3047 | O    | LEU | 83 | 10.481 | 24.402 | -11.107 | 1.00 | 23.84 |
| ATOM | 3048 | CB   | LEU | 83 | 10.640 | 27.258 | -9.919  | 1.00 | 21.97 |
| ATOM | 3049 | CG   | LEU | 83 | 10.183 | 28.361 | -8.970  | 1.00 | 22.43 |
| ATOM | 3050 | CD1  | LEU | 83 | 11.392 | 29.007 | -8.320  | 1.00 | 22.99 |
| ATOM | 3051 | CD2  | LEU | 83 | 9.388  | 29.397 | -9.730  | 1.00 | 24.38 |
| ATOM | 3052 | H    | LEU | 83 | 8.716  | 25.397 | -9.304  | 1.00 | 0.00  |
| ATOM | 3053 | N    | PRO | 84 | 10.445 | 25.739 | -12.923 | 1.00 | 24.83 |
| ATOM | 3054 | CA   | PRO | 84 | 11.064 | 24.737 | -13.788 | 1.00 | 25.04 |
| ATOM | 3055 | C    | PRO | 84 | 12.568 | 24.606 | -13.539 | 1.00 | 26.70 |
| ATOM | 3056 | O    | PRO | 84 | 13.240 | 25.567 | -13.143 | 1.00 | 26.43 |
| ATOM | 3057 | CB   | PRO | 84 | 10.771 | 25.273 | -15.183 | 1.00 | 24.05 |
| ATOM | 3058 | CG   | PRO | 84 | 10.820 | 26.734 | -14.987 | 1.00 | 24.45 |
| ATOM | 3059 | CD   | PRO | 84 | 10.036 | 26.914 | -13.711 | 1.00 | 25.04 |
| ATOM | 3060 | N    | VAL | 85 | 13.069 | 23.395 | -13.763 | 1.00 | 27.88 |
| ATOM | 3061 | CA   | VAL | 85 | 14.474 | 23.050 | -13.597 | 1.00 | 26.80 |
| ATOM | 3062 | C    | VAL | 85 | 15.106 | 22.978 | -14.981 | 1.00 | 27.62 |
| ATOM | 3063 | O    | VAL | 85 | 14.478 | 22.512 | -15.931 | 1.00 | 29.02 |
| ATOM | 3064 | CB   | VAL | 85 | 14.603 | 21.677 | -12.927 | 1.00 | 25.93 |
| ATOM | 3065 | CG1  | VAL | 85 | 16.045 | 21.216 | -12.923 | 1.00 | 26.71 |
| ATOM | 3066 | CG2  | VAL | 85 | 14.057 | 21.743 | -11.517 | 1.00 | 27.01 |
| ATOM | 3067 | H    | VAL | 85 | 12.479 | 22.686 | -14.091 | 1.00 | 0.00  |

|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 3068 | N    | SER | 86 | 16.357 | 23.401 | -15.089 | 1.00 | 27.09 |
| ATOM | 3069 | CA   | SER | 86 | 17.052 | 23.383 | -16.365 | 1.00 | 26.70 |
| ATOM | 3070 | C    | SER | 86 | 18.112 | 22.297 | -16.434 | 1.00 | 26.19 |
| ATOM | 3071 | O    | SER | 86 | 18.439 | 21.788 | -17.516 | 1.00 | 27.64 |
| ATOM | 3072 | CB   | SER | 86 | 17.690 | 24.743 | -16.619 | 1.00 | 27.96 |
| ATOM | 3073 | OG   | SER | 86 | 18.409 | 25.162 | -15.478 | 1.00 | 30.97 |
| ATOM | 3074 | H    | SER | 86 | 16.834 | 23.716 | -14.302 | 1.00 | 0.00  |
| ATOM | 3075 | HG   | SER | 86 | 18.180 | 26.055 | -15.190 | 1.00 | 0.00  |
| ATOM | 3076 | N    | ARG | 87 | 18.625 | 21.900 | -15.281 | 1.00 | 24.37 |
| ATOM | 3077 | CA   | ARG | 87 | 19.661 | 20.893 | -15.286 | 1.00 | 23.98 |
| ATOM | 3078 | C    | ARG | 87 | 19.688 | 20.201 | -13.942 | 1.00 | 21.85 |
| ATOM | 3079 | O    | ARG | 87 | 19.490 | 20.841 | -12.912 | 1.00 | 21.59 |
| ATOM | 3080 | CB   | ARG | 87 | 20.990 | 21.593 | -15.587 | 1.00 | 26.89 |
| ATOM | 3081 | CG   | ARG | 87 | 22.136 | 20.709 | -16.036 | 1.00 | 29.45 |
| ATOM | 3082 | CD   | ARG | 87 | 23.149 | 21.515 | -16.846 | 1.00 | 29.90 |
| ATOM | 3083 | NE   | ARG | 87 | 23.399 | 22.830 | -16.267 | 1.00 | 30.32 |
| ATOM | 3084 | CZ   | ARG | 87 | 24.595 | 23.284 | -15.904 | 1.00 | 30.98 |
| ATOM | 3085 | NH1  | ARG | 87 | 25.672 | 22.524 | -16.059 | 1.00 | 30.98 |
| ATOM | 3086 | NH2  | ARG | 87 | 24.707 | 24.499 | -15.372 | 1.00 | 30.47 |
| ATOM | 3087 | H    | ARG | 87 | 18.353 | 22.309 | -14.434 | 1.00 | 0.00  |
| ATOM | 3088 | HE   | ARG | 87 | 22.628 | 23.433 | -16.122 | 1.00 | 0.00  |
| ATOM | 3089 | HH11 | ARG | 87 | 25.618 | 21.608 | -16.475 | 1.00 | 0.00  |
| ATOM | 3090 | HH12 | ARG | 87 | 26.589 | 22.864 | -15.797 | 1.00 | 0.00  |
| ATOM | 3091 | HH21 | ARG | 87 | 23.869 | 25.063 | -15.222 | 1.00 | 0.00  |
| ATOM | 3092 | HH22 | ARG | 87 | 25.564 | 24.907 | -15.064 | 1.00 | 0.00  |
| ATOM | 3093 | N    | ILE | 88 | 19.850 | 18.884 | -13.969 | 1.00 | 20.50 |
| ATOM | 3094 | CA   | ILE | 88 | 19.913 | 18.066 | -12.759 | 1.00 | 22.18 |
| ATOM | 3095 | C    | ILE | 88 | 21.308 | 17.445 | -12.703 | 1.00 | 23.46 |
| ATOM | 3096 | O    | ILE | 88 | 21.732 | 16.771 | -13.644 | 1.00 | 24.82 |
| ATOM | 3097 | CB   | ILE | 88 | 18.859 | 16.913 | -12.780 | 1.00 | 22.63 |
| ATOM | 3098 | CG1  | ILE | 88 | 17.438 | 17.481 | -12.817 | 1.00 | 23.16 |
| ATOM | 3099 | CG2  | ILE | 88 | 19.027 | 15.995 | -11.572 | 1.00 | 20.50 |
| ATOM | 3100 | H    | ILE | 88 | 19.953 | 18.439 | -14.842 | 1.00 | 0.00  |
| ATOM | 3101 | CD   | ILE | 88 | 16.370 | 16.419 | -12.796 | 1.00 | 24.85 |
| ATOM | 3102 | N    | ILE | 89 | 22.032 | 17.687 | -11.620 | 1.00 | 23.34 |
| ATOM | 3103 | CA   | ILE | 89 | 23.373 | 17.139 | -11.481 | 1.00 | 22.63 |
| ATOM | 3104 | C    | ILE | 89 | 23.463 | 16.186 | -10.300 | 1.00 | 22.23 |
| ATOM | 3105 | O    | ILE | 89 | 23.388 | 16.596 | -9.140  | 1.00 | 22.16 |
| ATOM | 3106 | CB   | ILE | 89 | 24.425 | 18.255 | -11.399 | 1.00 | 22.65 |
| ATOM | 3107 | CG1  | ILE | 89 | 24.535 | 18.926 | -12.769 | 1.00 | 22.29 |
| ATOM | 3108 | CG2  | ILE | 89 | 25.770 | 17.695 | -10.969 | 1.00 | 22.49 |
| ATOM | 3109 | H    | ILE | 89 | 21.661 | 18.228 | -10.916 | 1.00 | 0.00  |
| ATOM | 3110 | CD   | ILE | 89 | 25.457 | 20.087 | -12.806 | 1.00 | 25.72 |
| ATOM | 3111 | N    | VAL | 90 | 23.561 | 14.901 | -10.629 | 1.00 | 21.11 |
| ATOM | 3112 | CA   | VAL | 90 | 23.642 | 13.825 | -9.652  | 1.00 | 18.37 |
| ATOM | 3113 | C    | VAL | 90 | 25.093 | 13.402 | -9.491  | 1.00 | 16.51 |
| ATOM | 3114 | O    | VAL | 90 | 25.788 | 13.168 | -10.480 | 1.00 | 14.67 |
| ATOM | 3115 | CB   | VAL | 90 | 22.807 | 12.613 | -10.112 | 1.00 | 17.30 |
| ATOM | 3116 | CG1  | VAL | 90 | 22.950 | 11.458 | -9.139  | 1.00 | 19.21 |
| ATOM | 3117 | CG2  | VAL | 90 | 21.356 | 13.007 | -10.240 | 1.00 | 17.04 |
| ATOM | 3118 | H    | VAL | 90 | 23.611 | 14.677 | -11.581 | 1.00 | 0.00  |
| ATOM | 3119 | N    | HIS | 91 | 25.550 | 13.323 | -8.245  | 1.00 | 14.91 |
| ATOM | 3120 | CA   | HIS | 91 | 26.912 | 12.927 | -7.984  | 1.00 | 14.56 |
| ATOM | 3121 | C    | HIS | 91 | 27.140 | 11.568 | -8.620  | 1.00 | 16.19 |
| ATOM | 3122 | O    | HIS | 91 | 26.495 | 10.587 | -8.261  | 1.00 | 17.08 |
| ATOM | 3123 | CB   | HIS | 91 | 27.180 | 12.852 | -6.491  | 1.00 | 14.24 |
| ATOM | 3124 | CG   | HIS | 91 | 28.632 | 12.716 | -6.158  | 1.00 | 13.82 |
| ATOM | 3125 | ND1  | HIS | 91 | 29.425 | 13.794 | -5.824  | 1.00 | 14.00 |
| ATOM | 3126 | CD2  | HIS | 91 | 29.446 | 11.635 | -6.144  | 1.00 | 12.66 |
| ATOM | 3127 | CE1  | HIS | 91 | 30.661 | 13.384 | -5.618  | 1.00 | 12.98 |
| ATOM | 3128 | NE2  | HIS | 91 | 30.700 | 12.078 | -5.807  | 1.00 | 13.51 |
| ATOM | 3129 | H    | HIS | 91 | 24.957 | 13.508 | -7.484  | 1.00 | 0.00  |
| ATOM | 3130 | HD1  | HIS | 91 | 29.117 | 14.726 | -5.748  | 1.00 | 0.00  |

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|      |      |      |     |    |        |        |         |      |       |
|------|------|------|-----|----|--------|--------|---------|------|-------|
| ATOM | 3131 | HE2  | HIS | 91 | 31.515 | 11.538 | -5.714  | 1.00 | 0.00  |
| ATOM | 3132 | N    | PRO | 92 | 28.130 | 11.478 | -9.513  | 1.00 | 17.82 |
| ATOM | 3133 | CA   | PRO | 92 | 28.496 | 10.255 | -10.239 | 1.00 | 17.81 |
| ATOM | 3134 | C    | PRO | 92 | 28.666 | 8.970  | -9.442  | 1.00 | 17.65 |
| ATOM | 3135 | O    | PRO | 92 | 28.420 | 7.893  | -9.970  | 1.00 | 19.34 |
| ATOM | 3136 | CB   | PRO | 92 | 29.791 | 10.648 | -10.956 | 1.00 | 17.26 |
| ATOM | 3137 | CG   | PRO | 92 | 30.326 | 11.790 | -10.127 | 1.00 | 18.76 |
| ATOM | 3138 | CD   | PRO | 92 | 29.086 | 12.560 | -9.803  | 1.00 | 18.30 |
| ATOM | 3139 | N    | GLN | 93 | 29.092 | 9.065  | -8.190  | 1.00 | 17.14 |
| ATOM | 3140 | CA   | GLN | 93 | 29.292 | 7.863  | -7.392  | 1.00 | 18.42 |
| ATOM | 3141 | C    | GLN | 93 | 28.035 | 7.359  | -6.739  | 1.00 | 18.03 |
| ATOM | 3142 | O    | GLN | 93 | 28.070 | 6.372  | -6.005  | 1.00 | 19.16 |
| ATOM | 3143 | CB   | GLN | 93 | 30.350 | 8.084  | -6.318  | 1.00 | 22.02 |
| ATOM | 3144 | CG   | GLN | 93 | 31.728 | 8.382  | -6.864  | 1.00 | 28.17 |
| ATOM | 3145 | CD   | GLN | 93 | 32.828 | 7.919  | -5.935  | 1.00 | 31.41 |
| ATOM | 3146 | OE1  | GLN | 93 | 33.531 | 6.946  | -6.227  | 1.00 | 33.61 |
| ATOM | 3147 | NE2  | GLN | 93 | 32.981 | 8.605  | -4.804  | 1.00 | 32.92 |
| ATOM | 3148 | H    | GLN | 93 | 29.242 | 9.942  | -7.818  | 1.00 | 0.00  |
| ATOM | 3149 | HE21 | GLN | 93 | 32.406 | 9.350  | -4.576  | 1.00 | 0.00  |
| ATOM | 3150 | HE22 | GLN | 93 | 33.719 | 8.285  | -4.245  | 1.00 | 0.00  |
| ATOM | 3151 | N    | PHE | 94 | 26.922 | 8.030  | -6.995  | 1.00 | 17.80 |
| ATOM | 3152 | CA   | PHE | 94 | 25.674 | 7.621  | -6.389  | 1.00 | 17.79 |
| ATOM | 3153 | C    | PHE | 94 | 24.954 | 6.511  | -7.102  | 1.00 | 17.90 |
| ATOM | 3154 | O    | PHE | 94 | 24.847 | 6.509  | -8.322  | 1.00 | 19.86 |
| ATOM | 3155 | CB   | PHE | 94 | 24.700 | 8.786  | -6.259  | 1.00 | 18.50 |
| ATOM | 3156 | CG   | PHE | 94 | 23.375 | 8.384  | -5.676  | 1.00 | 20.01 |
| ATOM | 3157 | CD1  | PHE | 94 | 23.276 | 8.011  | -4.336  | 1.00 | 20.50 |
| ATOM | 3158 | CD2  | PHE | 94 | 22.238 | 8.316  | -6.472  | 1.00 | 21.38 |
| ATOM | 3159 | CE1  | PHE | 94 | 22.073 | 7.571  | -3.803  | 1.00 | 19.68 |
| ATOM | 3160 | CE2  | PHE | 94 | 21.025 | 7.876  | -5.942  | 1.00 | 21.21 |
| ATOM | 3161 | CZ   | PHE | 94 | 20.949 | 7.504  | -4.606  | 1.00 | 20.25 |
| ATOM | 3162 | H    | PHE | 94 | 26.870 | 8.777  | -7.617  | 1.00 | 0.00  |
| ATOM | 3163 | N    | TYR | 95 | 24.429 | 5.587  | -6.312  | 1.00 | 18.03 |
| ATOM | 3164 | CA   | TYR | 95 | 23.629 | 4.479  | -6.813  | 1.00 | 18.49 |
| ATOM | 3165 | C    | TYR | 95 | 22.711 | 3.996  | -5.689  | 1.00 | 17.84 |
| ATOM | 3166 | O    | TYR | 95 | 21.598 | 3.548  | -5.936  | 1.00 | 19.19 |
| ATOM | 3167 | CB   | TYR | 95 | 24.473 | 3.310  | -7.346  | 1.00 | 20.03 |
| ATOM | 3168 | CG   | TYR | 95 | 23.590 | 2.189  | -7.867  | 1.00 | 22.55 |
| ATOM | 3169 | CD1  | TYR | 95 | 22.914 | 2.313  | -9.086  | 1.00 | 23.53 |
| ATOM | 3170 | CD2  | TYR | 95 | 23.324 | 1.063  | -7.085  | 1.00 | 22.97 |
| ATOM | 3171 | CE1  | TYR | 95 | 21.986 | 1.352  | -9.506  | 1.00 | 23.67 |
| ATOM | 3172 | CE2  | TYR | 95 | 22.397 | 0.098  | -7.495  | 1.00 | 23.89 |
| ATOM | 3173 | CZ   | TYR | 95 | 21.730 | 0.251  | -8.702  | 1.00 | 24.25 |
| ATOM | 3174 | OH   | TYR | 95 | 20.796 | -0.688 | -9.082  | 1.00 | 25.15 |
| ATOM | 3175 | H    | TYR | 95 | 24.612 | 5.705  | -5.360  | 1.00 | 0.00  |
| ATOM | 3176 | HH   | TYR | 95 | 20.347 | -0.398 | -9.893  | 1.00 | 0.00  |
| ATOM | 3177 | N    | THR | 96 | 23.174 | 4.120  | -4.451  | 1.00 | 16.68 |
| ATOM | 3178 | CA   | THR | 96 | 22.410 | 3.696  | -3.289  | 1.00 | 14.87 |
| ATOM | 3179 | C    | THR | 96 | 22.768 | 4.584  | -2.106  | 1.00 | 15.76 |
| ATOM | 3180 | O    | THR | 96 | 23.901 | 5.050  | -1.991  | 1.00 | 16.26 |
| ATOM | 3181 | CB   | THR | 96 | 22.732 | 2.229  | -2.947  | 1.00 | 14.73 |
| ATOM | 3182 | OG1  | THR | 96 | 21.909 | 1.357  | -3.725  | 1.00 | 16.07 |
| ATOM | 3183 | CG2  | THR | 96 | 22.526 | 1.948  | -1.499  | 1.00 | 14.86 |
| ATOM | 3184 | H    | THR | 96 | 24.069 | 4.484  | -4.291  | 1.00 | 0.00  |
| ATOM | 3185 | HG1  | THR | 96 | 20.987 | 1.624  | -3.669  | 1.00 | 0.00  |
| ATOM | 3186 | N    | ALA | 97 | 21.799 | 4.816  | -1.229  | 1.00 | 16.38 |
| ATOM | 3187 | CA   | ALA | 97 | 22.018 | 5.638  | -0.048  | 1.00 | 16.61 |
| ATOM | 3188 | C    | ALA | 97 | 23.063 | 5.003  | 0.871   | 1.00 | 18.45 |
| ATOM | 3189 | O    | ALA | 97 | 24.058 | 5.629  | 1.208   | 1.00 | 20.27 |
| ATOM | 3190 | CB   | ALA | 97 | 20.715 | 5.828  | 0.698   | 1.00 | 16.35 |
| ATOM | 3191 | H    | ALA | 97 | 20.919 | 4.418  | -1.380  | 1.00 | 0.00  |
| ATOM | 3192 | N    | GLN | 98 | 22.862 | 3.734  | 1.220   | 1.00 | 20.21 |
| ATOM | 3193 | CA   | GLN | 98 | 23.764 | 2.996  | 2.117   | 1.00 | 21.87 |

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|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3194 | C    | GLN | 98  | 25.193 | 2.980  | 1.597  | 1.00 | 20.81 |
| ATOM | 3195 | O    | GLN | 98  | 26.151 | 2.835  | 2.361  | 1.00 | 19.93 |
| ATOM | 3196 | CB   | GLN | 98  | 23.295 | 1.544  | 2.297  | 1.00 | 24.44 |
| ATOM | 3197 | CG   | GLN | 98  | 21.982 | 1.371  | 3.035  | 1.00 | 27.69 |
| ATOM | 3198 | CD   | GLN | 98  | 20.818 | 2.007  | 2.311  | 1.00 | 30.78 |
| ATOM | 3199 | OE1  | GLN | 98  | 20.808 | 2.094  | 1.084  | 1.00 | 31.89 |
| ATOM | 3200 | NE2  | GLN | 98  | 19.836 | 2.476  | 3.066  | 1.00 | 33.22 |
| ATOM | 3201 | H    | GLN | 98  | 22.113 | 3.291  | 0.794  | 1.00 | 0.00  |
| ATOM | 3202 | HE21 | GLN | 98  | 19.928 | 2.360  | 4.032  | 1.00 | 0.00  |
| ATOM | 3203 | HE22 | GLN | 98  | 19.073 | 2.895  | 2.610  | 1.00 | 0.00  |
| ATOM | 3204 | N    | ILE | 99  | 25.317 | 3.046  | 0.280  | 1.00 | 20.30 |
| ATOM | 3205 | CA   | ILE | 99  | 26.611 | 3.052  | -0.358 | 1.00 | 21.90 |
| ATOM | 3206 | C    | ILE | 99  | 27.280 | 4.406  | -0.124 | 1.00 | 23.75 |
| ATOM | 3207 | O    | ILE | 99  | 28.421 | 4.453  | 0.332  | 1.00 | 26.39 |
| ATOM | 3208 | CB   | ILE | 99  | 26.480 | 2.689  | -1.850 | 1.00 | 21.91 |
| ATOM | 3209 | CG1  | ILE | 99  | 26.382 | 1.166  | -1.985 | 1.00 | 21.54 |
| ATOM | 3210 | CG2  | ILE | 99  | 27.633 | 3.255  | -2.653 | 1.00 | 24.65 |
| ATOM | 3211 | H    | ILE | 99  | 24.518 | 3.118  | -0.269 | 1.00 | 0.00  |
| ATOM | 3212 | CD   | ILE | 99  | 26.231 | 0.657  | -3.394 | 1.00 | 19.95 |
| ATOM | 3213 | N    | GLY | 100 | 26.570 | 5.498  | -0.401 | 1.00 | 23.83 |
| ATOM | 3214 | CA   | GLY | 100 | 27.129 | 6.822  | -0.174 | 1.00 | 21.64 |
| ATOM | 3215 | C    | GLY | 100 | 26.976 | 7.786  | -1.333 | 1.00 | 20.52 |
| ATOM | 3216 | O    | GLY | 100 | 26.308 | 7.494  | -2.325 | 1.00 | 19.73 |
| ATOM | 3217 | H    | GLY | 100 | 25.683 | 5.438  | -0.817 | 1.00 | 0.00  |
| ATOM | 3218 | N    | ALA | 101 | 27.577 | 8.960  | -1.186 | 1.00 | 20.72 |
| ATOM | 3219 | CA   | ALA | 101 | 27.542 | 9.994  | -2.211 | 1.00 | 20.27 |
| ATOM | 3220 | C    | ALA | 101 | 26.154 | 10.540 | -2.481 | 1.00 | 19.41 |
| ATOM | 3221 | O    | ALA | 101 | 25.931 | 11.192 | -3.496 | 1.00 | 21.65 |
| ATOM | 3222 | CB   | ALA | 101 | 28.158 | 9.477  | -3.505 | 1.00 | 19.99 |
| ATOM | 3223 | H    | ALA | 101 | 28.094 | 9.152  | -0.370 | 1.00 | 0.00  |
| ATOM | 3224 | N    | ASP | 102 | 25.240 | 10.343 | -1.544 | 1.00 | 17.49 |
| ATOM | 3225 | CA   | ASP | 102 | 23.873 | 10.806 | -1.724 | 1.00 | 15.51 |
| ATOM | 3226 | C    | ASP | 102 | 23.738 | 12.320 | -1.696 | 1.00 | 15.17 |
| ATOM | 3227 | O    | ASP | 102 | 23.385 | 12.902 | -0.676 | 1.00 | 15.11 |
| ATOM | 3228 | CB   | ASP | 102 | 22.974 | 10.197 | -0.660 | 1.00 | 15.37 |
| ATOM | 3229 | CG   | ASP | 102 | 21.526 | 10.219 | -1.048 | 1.00 | 16.45 |
| ATOM | 3230 | OD1  | ASP | 102 | 21.174 | 10.789 | -2.096 | 1.00 | 16.31 |
| ATOM | 3231 | OD2  | ASP | 102 | 20.719 | 9.642  | -0.306 | 1.00 | 19.62 |
| ATOM | 3232 | H    | ASP | 102 | 25.491 | 9.899  | -0.710 | 1.00 | 0.00  |
| ATOM | 3233 | N    | ILE | 103 | 23.992 | 12.957 | -2.829 | 1.00 | 14.64 |
| ATOM | 3234 | CA   | ILE | 103 | 23.890 | 14.404 | -2.921 | 1.00 | 14.84 |
| ATOM | 3235 | C    | ILE | 103 | 23.626 | 14.746 | -4.389 | 1.00 | 15.54 |
| ATOM | 3236 | O    | ILE | 103 | 24.140 | 14.065 | -5.292 | 1.00 | 15.63 |
| ATOM | 3237 | CB   | ILE | 103 | 25.195 | 15.082 | -2.384 | 1.00 | 15.38 |
| ATOM | 3238 | CG1  | ILE | 103 | 24.935 | 16.540 | -1.988 | 1.00 | 14.76 |
| ATOM | 3239 | CG2  | ILE | 103 | 26.327 | 14.967 | -3.404 | 1.00 | 14.78 |
| ATOM | 3240 | H    | ILE | 103 | 24.286 | 12.439 | -3.609 | 1.00 | 0.00  |
| ATOM | 3241 | CD   | ILE | 103 | 26.094 | 17.201 | -1.268 | 1.00 | 11.34 |
| ATOM | 3242 | N    | ALA | 104 | 22.785 | 15.753 | -4.623 | 1.00 | 15.37 |
| ATOM | 3243 | CA   | ALA | 104 | 22.428 | 16.178 | -5.976 | 1.00 | 15.05 |
| ATOM | 3244 | C    | ALA | 104 | 22.124 | 17.660 | -6.019 | 1.00 | 15.32 |
| ATOM | 3245 | O    | ALA | 104 | 21.809 | 18.263 | -4.996 | 1.00 | 16.76 |
| ATOM | 3246 | CB   | ALA | 104 | 21.236 | 15.399 | -6.472 | 1.00 | 15.24 |
| ATOM | 3247 | H    | ALA | 104 | 22.358 | 16.234 | -3.890 | 1.00 | 0.00  |
| ATOM | 3248 | N    | LEU | 105 | 22.200 | 18.228 | -7.215 | 1.00 | 15.71 |
| ATOM | 3249 | CA   | LEU | 105 | 21.960 | 19.646 | -7.442 | 1.00 | 17.31 |
| ATOM | 3250 | C    | LEU | 105 | 20.948 | 19.862 | -8.561 | 1.00 | 19.06 |
| ATOM | 3251 | O    | LEU | 105 | 21.033 | 19.222 | -9.611 | 1.00 | 19.06 |
| ATOM | 3252 | CB   | LEU | 105 | 23.262 | 20.328 | -7.868 | 1.00 | 17.05 |
| ATOM | 3253 | CG   | LEU | 105 | 24.444 | 20.403 | -6.910 | 1.00 | 16.15 |
| ATOM | 3254 | CD1  | LEU | 105 | 25.683 | 20.853 | -7.669 | 1.00 | 15.03 |
| ATOM | 3255 | CD2  | LEU | 105 | 24.113 | 21.362 | -5.777 | 1.00 | 16.80 |
| ATOM | 3256 | H    | LEU | 105 | 22.468 | 17.677 | -7.971 | 1.00 | 0.00  |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 3257 | N   | LEU | 106 | 20.015 | 20.784 | -8.354  | 1.00 | 18.81 |
| ATOM | 3258 | CA  | LEU | 106 | 19.022 | 21.095 | -9.369  | 1.00 | 18.38 |
| ATOM | 3259 | C   | LEU | 106 | 19.249 | 22.552 | -9.721  | 1.00 | 19.95 |
| ATOM | 3260 | O   | LEU | 106 | 19.358 | 23.389 | -8.827  | 1.00 | 20.25 |
| ATOM | 3261 | CB  | LEU | 106 | 17.613 | 20.923 | -8.818  | 1.00 | 18.45 |
| ATOM | 3262 | CG  | LEU | 106 | 17.302 | 19.714 | -7.932  | 1.00 | 19.10 |
| ATOM | 3263 | CD1 | LEU | 106 | 15.795 | 19.581 | -7.795  | 1.00 | 19.66 |
| ATOM | 3264 | CD2 | LEU | 106 | 17.867 | 18.445 | -8.518  | 1.00 | 20.28 |
| ATOM | 3265 | H   | LEU | 106 | 20.026 | 21.246 | -7.491  | 1.00 | 0.00  |
| ATOM | 3266 | N   | GLU | 107 | 19.400 | 22.844 | -11.006 | 1.00 | 21.93 |
| ATOM | 3267 | CA  | GLU | 107 | 19.623 | 24.215 | -11.452 | 1.00 | 24.66 |
| ATOM | 3268 | C   | GLU | 107 | 18.293 | 24.778 | -11.904 | 1.00 | 25.13 |
| ATOM | 3269 | O   | GLU | 107 | 17.572 | 24.129 | -12.664 | 1.00 | 26.66 |
| ATOM | 3270 | CB  | GLU | 107 | 20.631 | 24.252 | -12.614 | 1.00 | 26.28 |
| ATOM | 3271 | CG  | GLU | 107 | 20.927 | 25.657 | -13.160 | 1.00 | 27.29 |
| ATOM | 3272 | CD  | GLU | 107 | 21.953 | 25.661 | -14.289 | 1.00 | 29.17 |
| ATOM | 3273 | OE1 | GLU | 107 | 22.959 | 26.386 | -14.187 | 1.00 | 30.52 |
| ATOM | 3274 | OE2 | GLU | 107 | 21.777 | 24.940 | -15.293 | 1.00 | 31.23 |
| ATOM | 3275 | H   | GLU | 107 | 19.378 | 22.140 | -11.669 | 1.00 | 0.00  |
| ATOM | 3276 | N   | LEU | 108 | 17.948 | 25.966 | -11.422 | 1.00 | 23.99 |
| ATOM | 3277 | CA  | LEU | 108 | 16.689 | 26.587 | -11.803 | 1.00 | 24.64 |
| ATOM | 3278 | C   | LEU | 108 | 16.868 | 27.234 | -13.171 | 1.00 | 29.15 |
| ATOM | 3279 | O   | LEU | 108 | 17.994 | 27.557 | -13.555 | 1.00 | 30.56 |
| ATOM | 3280 | CB  | LEU | 108 | 16.282 | 27.628 | -10.766 | 1.00 | 20.08 |
| ATOM | 3281 | CG  | LEU | 108 | 16.096 | 27.099 | -9.345  | 1.00 | 17.40 |
| ATOM | 3282 | CD1 | LEU | 108 | 15.604 | 28.210 | -8.446  | 1.00 | 17.94 |
| ATOM | 3283 | CD2 | LEU | 108 | 15.110 | 25.953 | -9.327  | 1.00 | 15.86 |
| ATOM | 3284 | H   | LEU | 108 | 18.597 | 26.433 | -10.858 | 1.00 | 0.00  |
| ATOM | 3285 | N   | GLU | 109 | 15.783 | 27.393 | -13.925 | 1.00 | 34.05 |
| ATOM | 3286 | CA  | GLU | 109 | 15.878 | 28.014 | -15.249 | 1.00 | 39.14 |
| ATOM | 3287 | C   | GLU | 109 | 16.218 | 29.495 | -15.112 | 1.00 | 41.66 |
| ATOM | 3288 | O   | GLU | 109 | 16.942 | 30.053 | -15.934 | 1.00 | 42.60 |
| ATOM | 3289 | CB  | GLU | 109 | 14.579 | 27.842 | -16.047 | 1.00 | 41.87 |
| ATOM | 3290 | CG  | GLU | 109 | 14.169 | 26.380 | -16.270 | 1.00 | 47.69 |
| ATOM | 3291 | CD  | GLU | 109 | 14.120 | 25.960 | -17.742 | 1.00 | 50.47 |
| ATOM | 3292 | OE1 | GLU | 109 | 13.324 | 25.050 | -18.074 | 1.00 | 51.05 |
| ATOM | 3293 | OE2 | GLU | 109 | 14.887 | 26.517 | -18.561 | 1.00 | 51.80 |
| ATOM | 3294 | H   | GLU | 109 | 14.908 | 27.060 | -13.609 | 1.00 | 0.00  |
| ATOM | 3295 | N   | GLU | 110 | 15.729 | 30.114 | -14.045 | 1.00 | 44.14 |
| ATOM | 3296 | CA  | GLU | 110 | 15.978 | 31.528 | -13.784 | 1.00 | 47.55 |
| ATOM | 3297 | C   | GLU | 110 | 16.286 | 31.701 | -12.299 | 1.00 | 48.50 |
| ATOM | 3298 | O   | GLU | 110 | 15.821 | 30.916 | -11.467 | 1.00 | 49.30 |
| ATOM | 3299 | CB  | GLU | 110 | 14.744 | 32.357 | -14.154 | 1.00 | 50.55 |
| ATOM | 3300 | CG  | GLU | 110 | 13.481 | 31.919 | -13.414 | 1.00 | 54.94 |
| ATOM | 3301 | CD  | GLU | 110 | 12.254 | 32.729 | -13.785 | 1.00 | 56.79 |
| ATOM | 3302 | OE1 | GLU | 110 | 11.801 | 33.542 | -12.950 | 1.00 | 58.86 |
| ATOM | 3303 | OE2 | GLU | 110 | 11.732 | 32.540 | -14.904 | 1.00 | 57.42 |
| ATOM | 3304 | H   | GLU | 110 | 15.183 | 29.613 | -13.398 | 1.00 | 0.00  |
| ATOM | 3305 | N   | PRO | 111 | 17.128 | 32.687 | -11.952 | 1.00 | 48.50 |
| ATOM | 3306 | CA  | PRO | 111 | 17.479 | 32.931 | -10.550 | 1.00 | 48.59 |
| ATOM | 3307 | C   | PRO | 111 | 16.286 | 33.490 | -9.783  | 1.00 | 49.59 |
| ATOM | 3308 | O   | PRO | 111 | 15.459 | 34.215 | -10.342 | 1.00 | 49.69 |
| ATOM | 3309 | CB  | PRO | 111 | 18.594 | 33.971 | -10.653 | 1.00 | 48.14 |
| ATOM | 3310 | CG  | PRO | 111 | 19.174 | 33.734 | -12.013 | 1.00 | 48.12 |
| ATOM | 3311 | CD  | PRO | 111 | 17.945 | 33.522 | -12.845 | 1.00 | 48.37 |
| ATOM | 3312 | N   | VAL | 112 | 16.201 | 33.153 | -8.505  | 1.00 | 50.84 |
| ATOM | 3313 | CA  | VAL | 112 | 15.110 | 33.622 | -7.668  | 1.00 | 53.38 |
| ATOM | 3314 | C   | VAL | 112 | 15.533 | 34.865 | -6.901  | 1.00 | 56.72 |
| ATOM | 3315 | O   | VAL | 112 | 16.601 | 34.887 | -6.287  | 1.00 | 58.71 |
| ATOM | 3316 | CB  | VAL | 112 | 14.653 | 32.536 | -6.664  | 1.00 | 52.88 |
| ATOM | 3317 | CG1 | VAL | 112 | 14.176 | 31.304 | -7.407  | 1.00 | 53.74 |
| ATOM | 3318 | CG2 | VAL | 112 | 15.776 | 32.173 | -5.708  | 1.00 | 52.31 |
| ATOM | 3319 | H   | VAL | 112 | 16.926 | 32.607 | -8.142  | 1.00 | 0.00  |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3320 | N   | LYS | 113 | 14.722 | 35.917 | -6.970 | 1.00 | 58.96 |
| ATOM | 3321 | CA  | LYS | 113 | 15.022 | 37.152 | -6.248 | 1.00 | 60.41 |
| ATOM | 3322 | C   | LYS | 113 | 14.853 | 36.838 | -4.765 | 1.00 | 60.77 |
| ATOM | 3323 | O   | LYS | 113 | 13.757 | 36.967 | -4.216 | 1.00 | 61.43 |
| ATOM | 3324 | CB  | LYS | 113 | 14.057 | 38.276 | -6.647 | 1.00 | 61.58 |
| ATOM | 3325 | CG  | LYS | 113 | 13.890 | 38.485 | -8.147 | 1.00 | 63.29 |
| ATOM | 3326 | CD  | LYS | 113 | 12.543 | 37.954 | -8.629 | 1.00 | 65.05 |
| ATOM | 3327 | CE  | LYS | 113 | 11.376 | 38.698 | -7.973 | 1.00 | 65.70 |
| ATOM | 3328 | NZ  | LYS | 113 | 10.048 | 38.167 | -8.401 | 1.00 | 66.27 |
| ATOM | 3329 | H   | LYS | 113 | 13.925 | 35.825 | -7.520 | 1.00 | 0.00  |
| ATOM | 3330 | HZ1 | LYS | 113 | 9.962  | 37.166 | -8.136 | 1.00 | 0.00  |
| ATOM | 3331 | HZ2 | LYS | 113 | 9.955  | 38.272 | -9.432 | 1.00 | 0.00  |
| ATOM | 3332 | HZ3 | LYS | 113 | 9.304  | 38.717 | -7.925 | 1.00 | 0.00  |
| ATOM | 3333 | N   | VAL | 114 | 15.925 | 36.360 | -4.147 | 1.00 | 60.71 |
| ATOM | 3334 | CA  | VAL | 114 | 15.908 | 36.001 | -2.738 | 1.00 | 60.67 |
| ATOM | 3335 | C   | VAL | 114 | 15.500 | 37.157 | -1.829 | 1.00 | 60.65 |
| ATOM | 3336 | O   | VAL | 114 | 16.274 | 38.086 | -1.592 | 1.00 | 60.82 |
| ATOM | 3337 | CB  | VAL | 114 | 17.264 | 35.410 | -2.300 | 1.00 | 61.10 |
| ATOM | 3338 | CG1 | VAL | 114 | 17.445 | 34.025 | -2.915 | 1.00 | 61.42 |
| ATOM | 3339 | CG2 | VAL | 114 | 18.408 | 36.323 | -2.726 | 1.00 | 61.09 |
| ATOM | 3340 | H   | VAL | 114 | 16.737 | 36.214 | -4.674 | 1.00 | 0.00  |
| ATOM | 3341 | N   | SER | 115 | 14.267 | 37.102 | -1.340 | 1.00 | 61.08 |
| ATOM | 3342 | CA  | SER | 115 | 13.732 | 38.139 | -0.466 | 1.00 | 61.41 |
| ATOM | 3343 | C   | SER | 115 | 13.957 | 37.844 | 1.021  | 1.00 | 61.79 |
| ATOM | 3344 | O   | SER | 115 | 14.564 | 36.829 | 1.387  | 1.00 | 62.53 |
| ATOM | 3345 | CB  | SER | 115 | 12.238 | 38.347 | -0.752 | 1.00 | 60.84 |
| ATOM | 3346 | OG  | SER | 115 | 11.484 | 37.178 | -0.475 | 1.00 | 60.27 |
| ATOM | 3347 | H   | SER | 115 | 13.706 | 36.338 | -1.597 | 1.00 | 0.00  |
| ATOM | 3348 | HG  | SER | 115 | 11.199 | 37.174 | 0.429  | 1.00 | 0.00  |
| ATOM | 3349 | N   | SER | 116 | 13.436 | 38.720 | 1.876  | 1.00 | 61.44 |
| ATOM | 3350 | CA  | SER | 116 | 13.566 | 38.573 | 3.325  | 1.00 | 61.01 |
| ATOM | 3351 | C   | SER | 116 | 12.974 | 37.259 | 3.839  | 1.00 | 59.89 |
| ATOM | 3352 | O   | SER | 116 | 13.434 | 36.709 | 4.844  | 1.00 | 58.72 |
| ATOM | 3353 | CB  | SER | 116 | 12.889 | 39.756 | 4.028  | 1.00 | 61.11 |
| ATOM | 3354 | OG  | SER | 116 | 11.542 | 39.897 | 3.604  | 1.00 | 61.47 |
| ATOM | 3355 | H   | SER | 116 | 12.965 | 39.513 | 1.546  | 1.00 | 0.00  |
| ATOM | 3356 | HG  | SER | 116 | 11.260 | 40.769 | 3.917  | 1.00 | 0.00  |
| ATOM | 3357 | N   | HIS | 117 | 11.971 | 36.753 | 3.129  | 1.00 | 59.62 |
| ATOM | 3358 | CA  | HIS | 117 | 11.302 | 35.514 | 3.517  | 1.00 | 59.34 |
| ATOM | 3359 | C   | HIS | 117 | 11.737 | 34.297 | 2.695  | 1.00 | 56.48 |
| ATOM | 3360 | O   | HIS | 117 | 11.407 | 33.165 | 3.050  | 1.00 | 56.61 |
| ATOM | 3361 | CB  | HIS | 117 | 9.776  | 35.680 | 3.430  | 1.00 | 63.09 |
| ATOM | 3362 | CG  | HIS | 117 | 9.255  | 36.924 | 4.090  | 1.00 | 66.88 |
| ATOM | 3363 | ND1 | HIS | 117 | 9.417  | 37.184 | 5.436  | 1.00 | 67.62 |
| ATOM | 3364 | CD2 | HIS | 117 | 8.580  | 37.985 | 3.583  | 1.00 | 67.79 |
| ATOM | 3365 | CE1 | HIS | 117 | 8.866  | 38.349 | 5.728  | 1.00 | 68.20 |
| ATOM | 3366 | NE2 | HIS | 117 | 8.352  | 38.855 | 4.622  | 1.00 | 68.20 |
| ATOM | 3367 | H   | HIS | 117 | 11.705 | 37.219 | 2.318  | 1.00 | 0.00  |
| ATOM | 3368 | HD1 | HIS | 117 | 9.878  | 36.624 | 6.106  | 1.00 | 0.00  |
| ATOM | 3369 | HE2 | HIS | 117 | 7.875  | 39.714 | 4.550  | 1.00 | 0.00  |
| ATOM | 3370 | N   | VAL | 118 | 12.467 | 34.527 | 1.604  | 1.00 | 52.48 |
| ATOM | 3371 | CA  | VAL | 118 | 12.937 | 33.444 | 0.739  | 1.00 | 48.37 |
| ATOM | 3372 | C   | VAL | 118 | 14.356 | 33.705 | 0.246  | 1.00 | 46.52 |
| ATOM | 3373 | O   | VAL | 118 | 14.562 | 34.432 | -0.721 | 1.00 | 45.40 |
| ATOM | 3374 | CB  | VAL | 118 | 12.004 | 33.257 | -0.480 | 1.00 | 46.79 |
| ATOM | 3375 | CG1 | VAL | 118 | 12.673 | 32.415 | -1.553 | 1.00 | 46.40 |
| ATOM | 3376 | CG2 | VAL | 118 | 10.720 | 32.593 | -0.041 | 1.00 | 46.79 |
| ATOM | 3377 | H   | VAL | 118 | 12.723 | 35.429 | 1.328  | 1.00 | 0.00  |
| ATOM | 3378 | N   | HIS | 119 | 15.334 | 33.121 | 0.927  | 1.00 | 45.06 |
| ATOM | 3379 | CA  | HIS | 119 | 16.725 | 33.294 | 0.536  | 1.00 | 43.51 |
| ATOM | 3380 | C   | HIS | 119 | 17.584 | 32.079 | 0.860  | 1.00 | 41.34 |
| ATOM | 3381 | O   | HIS | 119 | 17.141 | 31.157 | 1.547  | 1.00 | 41.25 |
| ATOM | 3382 | CB  | HIS | 119 | 17.328 | 34.578 | 1.126  | 1.00 | 44.71 |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3383 | CG  | HIS | 119 | 17.256 | 34.664 | 2.618  | 1.00 | 45.16 |
| ATOM | 3384 | ND1 | HIS | 119 | 16.287 | 35.392 | 3.273  | 1.00 | 45.96 |
| ATOM | 3385 | CD2 | HIS | 119 | 18.054 | 34.148 | 3.582  | 1.00 | 46.03 |
| ATOM | 3386 | CE1 | HIS | 119 | 16.490 | 35.324 | 4.576  | 1.00 | 47.16 |
| ATOM | 3387 | NE2 | HIS | 119 | 17.558 | 34.575 | 4.790  | 1.00 | 47.71 |
| ATOM | 3388 | H   | HIS | 119 | 15.120 | 32.488 | 1.647  | 1.00 | 0.00  |
| ATOM | 3389 | HD1 | HIS | 119 | 15.585 | 35.902 | 2.803  | 1.00 | 0.00  |
| ATOM | 3390 | HE2 | HIS | 119 | 17.950 | 34.357 | 5.664  | 1.00 | 0.00  |
| ATOM | 3391 | N   | THR | 120 | 18.819 | 32.106 | 0.372  | 1.00 | 38.34 |
| ATOM | 3392 | CA  | THR | 120 | 19.766 | 31.013 | 0.541  | 1.00 | 34.55 |
| ATOM | 3393 | C   | THR | 120 | 20.300 | 30.749 | 1.943  | 1.00 | 32.22 |
| ATOM | 3394 | O   | THR | 120 | 20.341 | 31.640 | 2.790  | 1.00 | 33.28 |
| ATOM | 3395 | CB  | THR | 120 | 20.957 | 31.205 | -0.399 | 1.00 | 33.14 |
| ATOM | 3396 | OG1 | THR | 120 | 21.644 | 32.412 | -0.057 | 1.00 | 31.99 |
| ATOM | 3397 | CG2 | THR | 120 | 20.468 | 31.317 | -1.823 | 1.00 | 31.97 |
| ATOM | 3398 | H   | THR | 120 | 19.128 | 32.885 | -0.127 | 1.00 | 0.00  |
| ATOM | 3399 | HG1 | THR | 120 | 21.164 | 33.191 | -0.368 | 1.00 | 0.00  |
| ATOM | 3400 | N   | VAL | 121 | 20.679 | 29.497 | 2.181  | 1.00 | 29.15 |
| ATOM | 3401 | CA  | VAL | 121 | 21.254 | 29.085 | 3.452  | 1.00 | 27.82 |
| ATOM | 3402 | C   | VAL | 121 | 22.755 | 29.234 | 3.250  | 1.00 | 28.37 |
| ATOM | 3403 | O   | VAL | 121 | 23.207 | 29.538 | 2.145  | 1.00 | 28.69 |
| ATOM | 3404 | CB  | VAL | 121 | 20.902 | 27.613 | 3.795  | 1.00 | 26.96 |
| ATOM | 3405 | CG1 | VAL | 121 | 21.481 | 26.673 | 2.764  | 1.00 | 27.49 |
| ATOM | 3406 | CG2 | VAL | 121 | 21.379 | 27.247 | 5.196  | 1.00 | 24.97 |
| ATOM | 3407 | H   | VAL | 121 | 20.573 | 28.879 | 1.433  | 1.00 | 0.00  |
| ATOM | 3408 | N   | THR | 122 | 23.532 | 29.039 | 4.303  | 1.00 | 29.72 |
| ATOM | 3409 | CA  | THR | 122 | 24.969 | 29.171 | 4.183  | 1.00 | 31.59 |
| ATOM | 3410 | C   | THR | 122 | 25.618 | 27.802 | 4.349  | 1.00 | 32.19 |
| ATOM | 3411 | O   | THR | 122 | 25.270 | 27.053 | 5.269  | 1.00 | 32.90 |
| ATOM | 3412 | CB  | THR | 122 | 25.516 | 30.143 | 5.246  | 1.00 | 33.10 |
| ATOM | 3413 | OG1 | THR | 122 | 24.646 | 31.280 | 5.354  | 1.00 | 34.19 |
| ATOM | 3414 | CG2 | THR | 122 | 26.904 | 30.624 | 4.855  | 1.00 | 33.93 |
| ATOM | 3415 | H   | THR | 122 | 23.207 | 28.833 | 5.203  | 1.00 | 0.00  |
| ATOM | 3416 | HG1 | THR | 122 | 23.766 | 31.001 | 5.612  | 1.00 | 0.00  |
| ATOM | 3417 | N   | LEU | 123 | 26.515 | 27.452 | 3.430  | 1.00 | 31.53 |
| ATOM | 3418 | CA  | LEU | 123 | 27.209 | 26.167 | 3.496  | 1.00 | 31.02 |
| ATOM | 3419 | C   | LEU | 123 | 28.322 | 26.220 | 4.548  | 1.00 | 31.62 |
| ATOM | 3420 | O   | LEU | 123 | 29.049 | 27.204 | 4.661  | 1.00 | 32.50 |
| ATOM | 3421 | CB  | LEU | 123 | 27.773 | 25.771 | 2.121  | 1.00 | 29.42 |
| ATOM | 3422 | CG  | LEU | 123 | 26.790 | 25.351 | 1.019  | 1.00 | 26.99 |
| ATOM | 3423 | CD1 | LEU | 123 | 27.539 | 25.158 | -0.291 | 1.00 | 25.06 |
| ATOM | 3424 | CD2 | LEU | 123 | 26.053 | 24.076 | 1.416  | 1.00 | 24.67 |
| ATOM | 3425 | H   | LEU | 123 | 26.732 | 28.064 | 2.703  | 1.00 | 0.00  |
| ATOM | 3426 | N   | PRO | 124 | 28.448 | 25.164 | 5.354  | 1.00 | 32.64 |
| ATOM | 3427 | CA  | PRO | 124 | 29.466 | 25.094 | 6.400  | 1.00 | 34.01 |
| ATOM | 3428 | C   | PRO | 124 | 30.865 | 25.195 | 5.836  | 1.00 | 35.14 |
| ATOM | 3429 | O   | PRO | 124 | 31.122 | 24.755 | 4.725  | 1.00 | 34.65 |
| ATOM | 3430 | CB  | PRO | 124 | 29.232 | 23.711 | 6.998  | 1.00 | 33.70 |
| ATOM | 3431 | CG  | PRO | 124 | 28.733 | 22.933 | 5.818  | 1.00 | 32.32 |
| ATOM | 3432 | CD  | PRO | 124 | 27.740 | 23.882 | 5.238  | 1.00 | 32.80 |
| ATOM | 3433 | N   | PRO | 125 | 31.782 | 25.814 | 6.585  | 1.00 | 37.49 |
| ATOM | 3434 | CA  | PRO | 125 | 33.155 | 25.934 | 6.103  | 1.00 | 39.11 |
| ATOM | 3435 | C   | PRO | 125 | 33.768 | 24.534 | 6.072  | 1.00 | 40.69 |
| ATOM | 3436 | O   | PRO | 125 | 33.358 | 23.655 | 6.828  | 1.00 | 39.70 |
| ATOM | 3437 | CB  | PRO | 125 | 33.806 | 26.813 | 7.168  | 1.00 | 38.93 |
| ATOM | 3438 | CG  | PRO | 125 | 33.057 | 26.451 | 8.404  | 1.00 | 38.22 |
| ATOM | 3439 | CD  | PRO | 125 | 31.637 | 26.440 | 7.907  | 1.00 | 38.30 |
| ATOM | 3440 | N   | ALA | 126 | 34.750 | 24.340 | 5.202  | 1.00 | 43.31 |
| ATOM | 3441 | CA  | ALA | 126 | 35.410 | 23.048 | 5.054  | 1.00 | 46.91 |
| ATOM | 3442 | C   | ALA | 126 | 35.841 | 22.416 | 6.378  | 1.00 | 49.80 |
| ATOM | 3443 | O   | ALA | 126 | 35.583 | 21.238 | 6.633  | 1.00 | 49.92 |
| ATOM | 3444 | CB  | ALA | 126 | 36.606 | 23.185 | 4.121  | 1.00 | 47.29 |
| ATOM | 3445 | H   | ALA | 126 | 35.003 | 25.084 | 4.619  | 1.00 | 0.00  |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3446 | N   | SER | 127 | 36.471 | 23.220 | 7.228  | 1.00 | 52.56 |
| ATOM | 3447 | CA  | SER | 127 | 36.965 | 22.758 | 8.521  | 1.00 | 54.03 |
| ATOM | 3448 | C   | SER | 127 | 35.882 | 22.529 | 9.567  | 1.00 | 53.77 |
| ATOM | 3449 | O   | SER | 127 | 36.141 | 21.913 | 10.604 | 1.00 | 54.33 |
| ATOM | 3450 | CB  | SER | 127 | 38.012 | 23.748 | 9.062  | 1.00 | 55.86 |
| ATOM | 3451 | OG  | SER | 127 | 37.547 | 25.096 | 9.042  | 1.00 | 55.97 |
| ATOM | 3452 | H   | SER | 127 | 36.613 | 24.162 | 7.017  | 1.00 | 0.00  |
| ATOM | 3453 | HG  | SER | 127 | 36.899 | 25.219 | 9.754  | 1.00 | 0.00  |
| ATOM | 3454 | N   | GLU | 128 | 34.667 | 22.982 | 9.283  | 1.00 | 53.27 |
| ATOM | 3455 | CA  | GLU | 128 | 33.584 | 22.845 | 10.242 | 1.00 | 52.57 |
| ATOM | 3456 | C   | GLU | 128 | 33.379 | 21.431 | 10.738 | 1.00 | 51.46 |
| ATOM | 3457 | O   | GLU | 128 | 33.433 | 20.464 | 9.974  | 1.00 | 51.06 |
| ATOM | 3458 | CB  | GLU | 128 | 32.280 | 23.412 | 9.694  | 1.00 | 53.36 |
| ATOM | 3459 | CG  | GLU | 128 | 31.271 | 23.725 | 10.784 | 1.00 | 54.12 |
| ATOM | 3460 | CD  | GLU | 128 | 31.896 | 24.467 | 11.957 | 1.00 | 53.62 |
| ATOM | 3461 | OE1 | GLU | 128 | 32.412 | 25.586 | 11.755 | 1.00 | 53.92 |
| ATOM | 3462 | OE2 | GLU | 128 | 31.892 | 23.916 | 13.076 | 1.00 | 54.19 |
| ATOM | 3463 | H   | GLU | 128 | 34.461 | 23.358 | 8.410  | 1.00 | 0.00  |
| ATOM | 3464 | N   | THR | 129 | 33.158 | 21.330 | 12.039 | 1.00 | 50.59 |
| ATOM | 3465 | CA  | THR | 129 | 32.957 | 20.056 | 12.697 | 1.00 | 50.23 |
| ATOM | 3466 | C   | THR | 129 | 31.897 | 20.296 | 13.752 | 1.00 | 48.52 |
| ATOM | 3467 | O   | THR | 129 | 32.040 | 21.174 | 14.607 | 1.00 | 49.08 |
| ATOM | 3468 | CB  | THR | 129 | 34.258 | 19.566 | 13.375 | 1.00 | 51.98 |
| ATOM | 3469 | OG1 | THR | 129 | 35.310 | 19.488 | 12.403 | 1.00 | 52.92 |
| ATOM | 3470 | CG2 | THR | 129 | 34.047 | 18.191 | 14.005 | 1.00 | 53.49 |
| ATOM | 3471 | H   | THR | 129 | 33.075 | 22.147 | 12.589 | 1.00 | 0.00  |
| ATOM | 3472 | HG1 | THR | 129 | 35.517 | 20.322 | 11.951 | 1.00 | 0.00  |
| ATOM | 3473 | N   | PHE | 130 | 30.828 | 19.517 | 13.687 | 1.00 | 45.94 |
| ATOM | 3474 | CA  | PHE | 130 | 29.729 | 19.646 | 14.626 | 1.00 | 42.95 |
| ATOM | 3475 | C   | PHE | 130 | 29.930 | 18.670 | 15.774 | 1.00 | 41.42 |
| ATOM | 3476 | O   | PHE | 130 | 29.925 | 17.448 | 15.588 | 1.00 | 41.86 |
| ATOM | 3477 | CB  | PHE | 130 | 28.408 | 19.423 | 13.889 | 1.00 | 41.39 |
| ATOM | 3478 | CG  | PHE | 130 | 28.266 | 20.285 | 12.672 | 1.00 | 39.34 |
| ATOM | 3479 | CD1 | PHE | 130 | 29.033 | 20.029 | 11.535 | 1.00 | 38.47 |
| ATOM | 3480 | CD2 | PHE | 130 | 27.435 | 21.400 | 12.681 | 1.00 | 38.73 |
| ATOM | 3481 | CE1 | PHE | 130 | 28.977 | 20.874 | 10.429 | 1.00 | 38.13 |
| ATOM | 3482 | CE2 | PHE | 130 | 27.375 | 22.247 | 11.576 | 1.00 | 38.62 |
| ATOM | 3483 | CZ  | PHE | 130 | 28.149 | 21.985 | 10.452 | 1.00 | 37.77 |
| ATOM | 3484 | H   | PHE | 130 | 30.776 | 18.819 | 13.005 | 1.00 | 0.00  |
| ATOM | 3485 | N   | PRO | 131 | 30.188 | 19.205 | 16.974 | 1.00 | 39.65 |
| ATOM | 3486 | CA  | PRO | 131 | 30.415 | 18.422 | 18.191 | 1.00 | 39.34 |
| ATOM | 3487 | C   | PRO | 131 | 29.215 | 17.585 | 18.606 | 1.00 | 37.64 |
| ATOM | 3488 | O   | PRO | 131 | 28.074 | 18.028 | 18.509 | 1.00 | 36.77 |
| ATOM | 3489 | CB  | PRO | 131 | 30.736 | 19.497 | 19.230 | 1.00 | 40.21 |
| ATOM | 3490 | CG  | PRO | 131 | 29.932 | 20.666 | 18.755 | 1.00 | 40.85 |
| ATOM | 3491 | CD  | PRO | 131 | 30.192 | 20.647 | 17.272 | 1.00 | 39.74 |
| ATOM | 3492 | N   | PRO | 132 | 29.466 | 16.377 | 19.121 | 1.00 | 37.42 |
| ATOM | 3493 | CA  | PRO | 132 | 28.375 | 15.504 | 19.550 | 1.00 | 37.72 |
| ATOM | 3494 | C   | PRO | 132 | 27.533 | 16.249 | 20.565 | 1.00 | 38.37 |
| ATOM | 3495 | O   | PRO | 132 | 28.054 | 17.001 | 21.398 | 1.00 | 38.89 |
| ATOM | 3496 | CB  | PRO | 132 | 29.112 | 14.327 | 20.184 | 1.00 | 37.73 |
| ATOM | 3497 | CG  | PRO | 132 | 30.364 | 14.965 | 20.711 | 1.00 | 37.59 |
| ATOM | 3498 | CD  | PRO | 132 | 30.766 | 15.844 | 19.563 | 1.00 | 37.40 |
| ATOM | 3499 | N   | GLY | 133 | 26.225 | 16.077 | 20.479 | 1.00 | 39.47 |
| ATOM | 3500 | CA  | GLY | 133 | 25.351 | 16.763 | 21.399 | 1.00 | 41.19 |
| ATOM | 3501 | C   | GLY | 133 | 24.882 | 18.096 | 20.850 | 1.00 | 42.36 |
| ATOM | 3502 | O   | GLY | 133 | 23.771 | 18.519 | 21.172 | 1.00 | 44.14 |
| ATOM | 3503 | H   | GLY | 133 | 25.850 | 15.490 | 19.787 | 1.00 | 0.00  |
| ATOM | 3504 | N   | MET | 134 | 25.701 | 18.756 | 20.029 | 1.00 | 41.67 |
| ATOM | 3505 | CA  | MET | 134 | 25.311 | 20.043 | 19.455 | 1.00 | 41.10 |
| ATOM | 3506 | C   | MET | 134 | 23.939 | 19.873 | 18.821 | 1.00 | 41.05 |
| ATOM | 3507 | O   | MET | 134 | 23.740 | 19.000 | 17.968 | 1.00 | 41.93 |
| ATOM | 3508 | CB  | MET | 134 | 26.309 | 20.505 | 18.395 | 1.00 | 41.54 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3509 | CG  | MET | 134 | 25.883 | 21.760 | 17.658 | 1.00 | 43.25 |
| ATOM | 3510 | SD  | MET | 134 | 27.021 | 22.197 | 16.336 | 1.00 | 47.72 |
| ATOM | 3511 | CE  | MET | 134 | 27.509 | 23.857 | 16.830 | 1.00 | 47.53 |
| ATOM | 3512 | H   | MET | 134 | 26.553 | 18.382 | 19.728 | 1.00 | 0.00  |
| ATOM | 3513 | N   | PRO | 135 | 22.950 | 20.634 | 19.302 | 1.00 | 39.34 |
| ATOM | 3514 | CA  | PRO | 135 | 21.611 | 20.507 | 18.731 | 1.00 | 37.12 |
| ATOM | 3515 | C   | PRO | 135 | 21.502 | 21.224 | 17.398 | 1.00 | 34.98 |
| ATOM | 3516 | O   | PRO | 135 | 21.989 | 22.345 | 17.231 | 1.00 | 34.48 |
| ATOM | 3517 | CB  | PRO | 135 | 20.730 | 21.143 | 19.799 | 1.00 | 36.81 |
| ATOM | 3518 | CG  | PRO | 135 | 21.597 | 22.242 | 20.312 | 1.00 | 39.01 |
| ATOM | 3519 | CD  | PRO | 135 | 22.961 | 21.584 | 20.429 | 1.00 | 39.13 |
| ATOM | 3520 | N   | CYS | 136 | 20.911 | 20.537 | 16.439 | 1.00 | 33.50 |
| ATOM | 3521 | CA  | CYS | 136 | 20.695 | 21.083 | 15.117 | 1.00 | 32.45 |
| ATOM | 3522 | C   | CYS | 136 | 19.210 | 20.890 | 14.843 | 1.00 | 33.73 |
| ATOM | 3523 | O   | CYS | 136 | 18.495 | 20.337 | 15.684 | 1.00 | 34.39 |
| ATOM | 3524 | CB  | CYS | 136 | 21.544 | 20.335 | 14.098 | 1.00 | 30.37 |
| ATOM | 3525 | SG  | CYS | 136 | 23.334 | 20.503 | 14.358 | 1.00 | 26.22 |
| ATOM | 3526 | H   | CYS | 136 | 20.625 | 19.625 | 16.608 | 1.00 | 0.00  |
| ATOM | 3527 | N   | TRP | 137 | 18.738 | 21.344 | 13.686 | 1.00 | 33.94 |
| ATOM | 3528 | CA  | TRP | 137 | 17.324 | 21.224 | 13.342 | 1.00 | 33.40 |
| ATOM | 3529 | C   | TRP | 137 | 17.145 | 20.648 | 11.952 | 1.00 | 33.84 |
| ATOM | 3530 | O   | TRP | 137 | 17.884 | 21.003 | 11.037 | 1.00 | 35.74 |
| ATOM | 3531 | CB  | TRP | 137 | 16.656 | 22.600 | 13.352 | 1.00 | 33.55 |
| ATOM | 3532 | CG  | TRP | 137 | 16.834 | 23.404 | 14.600 | 1.00 | 32.89 |
| ATOM | 3533 | CD1 | TRP | 137 | 17.993 | 23.951 | 15.072 | 1.00 | 32.81 |
| ATOM | 3534 | CD2 | TRP | 137 | 15.809 | 23.789 | 15.512 | 1.00 | 33.22 |
| ATOM | 3535 | NE1 | TRP | 137 | 17.750 | 24.657 | 16.221 | 1.00 | 32.46 |
| ATOM | 3536 | CE2 | TRP | 137 | 16.416 | 24.575 | 16.515 | 1.00 | 32.62 |
| ATOM | 3537 | CE3 | TRP | 137 | 14.431 | 23.547 | 15.579 | 1.00 | 34.85 |
| ATOM | 3538 | CZ2 | TRP | 137 | 15.696 | 25.120 | 17.572 | 1.00 | 34.22 |
| ATOM | 3539 | CZ3 | TRP | 137 | 13.709 | 24.090 | 16.635 | 1.00 | 35.32 |
| ATOM | 3540 | CH2 | TRP | 137 | 14.345 | 24.869 | 17.617 | 1.00 | 35.81 |
| ATOM | 3541 | H   | TRP | 137 | 19.351 | 21.782 | 13.054 | 1.00 | 0.00  |
| ATOM | 3542 | HE1 | TRP | 137 | 18.442 | 25.193 | 16.667 | 1.00 | 0.00  |
| ATOM | 3543 | N   | VAL | 138 | 16.159 | 19.773 | 11.796 | 1.00 | 34.21 |
| ATOM | 3544 | CA  | VAL | 138 | 15.846 | 19.179 | 10.495 | 1.00 | 34.78 |
| ATOM | 3545 | C   | VAL | 138 | 14.489 | 19.779 | 10.144 | 1.00 | 35.19 |
| ATOM | 3546 | O   | VAL | 138 | 13.687 | 20.056 | 11.045 | 1.00 | 36.78 |
| ATOM | 3547 | CB  | VAL | 138 | 15.679 | 17.649 | 10.566 | 1.00 | 35.29 |
| ATOM | 3548 | CG1 | VAL | 138 | 15.790 | 17.049 | 9.182  | 1.00 | 35.55 |
| ATOM | 3549 | CG2 | VAL | 138 | 16.703 | 17.040 | 11.485 | 1.00 | 37.18 |
| ATOM | 3550 | H   | VAL | 138 | 15.622 | 19.557 | 12.586 | 1.00 | 0.00  |
| ATOM | 3551 | N   | THR | 139 | 14.216 | 19.972 | 8.859  | 1.00 | 33.49 |
| ATOM | 3552 | CA  | THR | 139 | 12.941 | 20.562 | 8.461  | 1.00 | 32.04 |
| ATOM | 3553 | C   | THR | 139 | 12.356 | 19.855 | 7.242  | 1.00 | 31.06 |
| ATOM | 3554 | O   | THR | 139 | 13.100 | 19.430 | 6.354  | 1.00 | 31.55 |
| ATOM | 3555 | CB  | THR | 139 | 13.110 | 22.066 | 8.140  | 1.00 | 32.20 |
| ATOM | 3556 | OG1 | THR | 139 | 14.107 | 22.641 | 8.995  | 1.00 | 32.70 |
| ATOM | 3557 | CG2 | THR | 139 | 11.811 | 22.795 | 8.374  | 1.00 | 34.44 |
| ATOM | 3558 | H   | THR | 139 | 14.870 | 19.715 | 8.173  | 1.00 | 0.00  |
| ATOM | 3559 | HG1 | THR | 139 | 14.890 | 22.078 | 8.934  | 1.00 | 0.00  |
| ATOM | 3560 | N   | GLY | 140 | 11.030 | 19.740 | 7.194  | 1.00 | 29.01 |
| ATOM | 3561 | CA  | GLY | 140 | 10.390 | 19.083 | 6.064  | 1.00 | 26.53 |
| ATOM | 3562 | C   | GLY | 140 | 8.877  | 19.000 | 6.153  | 1.00 | 24.44 |
| ATOM | 3563 | O   | GLY | 140 | 8.268  | 19.568 | 7.051  | 1.00 | 26.54 |
| ATOM | 3564 | H   | GLY | 140 | 10.475 | 20.083 | 7.932  | 1.00 | 0.00  |
| ATOM | 3565 | N   | TRP | 141 | 8.272  | 18.301 | 5.200  | 1.00 | 21.59 |
| ATOM | 3566 | CA  | TRP | 141 | 6.822  | 18.122 | 5.138  | 1.00 | 18.01 |
| ATOM | 3567 | C   | TRP | 141 | 6.544  | 16.627 | 5.042  | 1.00 | 17.35 |
| ATOM | 3568 | O   | TRP | 141 | 5.624  | 16.201 | 4.334  | 1.00 | 17.29 |
| ATOM | 3569 | CB  | TRP | 141 | 6.256  | 18.778 | 3.875  | 1.00 | 15.10 |
| ATOM | 3570 | CG  | TRP | 141 | 6.260  | 20.267 | 3.834  | 1.00 | 13.29 |
| ATOM | 3571 | CD1 | TRP | 141 | 5.328  | 21.097 | 4.379  | 1.00 | 13.90 |

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|      |      |      |     |     |       |        |        |      |       |
|------|------|------|-----|-----|-------|--------|--------|------|-------|
| ATOM | 3572 | CD2  | TRP | 141 | 7.169 | 21.107 | 3.106  | 1.00 | 12.66 |
| ATOM | 3573 | NE1  | TRP | 141 | 5.589 | 22.399 | 4.023  | 1.00 | 13.85 |
| ATOM | 3574 | CE2  | TRP | 141 | 6.712 | 22.434 | 3.244  | 1.00 | 11.73 |
| ATOM | 3575 | CE3  | TRP | 141 | 8.318 | 20.866 | 2.345  | 1.00 | 13.90 |
| ATOM | 3576 | CZ2  | TRP | 141 | 7.360 | 23.514 | 2.650  | 1.00 | 11.79 |
| ATOM | 3577 | CZ3  | TRP | 141 | 8.968 | 21.944 | 1.751  | 1.00 | 13.55 |
| ATOM | 3578 | CH2  | TRP | 141 | 8.486 | 23.250 | 1.909  | 1.00 | 13.61 |
| ATOM | 3579 | H    | TRP | 141 | 8.847 | 17.848 | 4.553  | 1.00 | 0.00  |
| ATOM | 3580 | HE1  | TRP | 141 | 5.064 | 23.185 | 4.278  | 1.00 | 0.00  |
| ATOM | 3581 | N    | GLY | 142 | 7.375 | 15.828 | 5.699  | 1.00 | 16.09 |
| ATOM | 3582 | CA   | GLY | 142 | 7.202 | 14.392 | 5.637  | 1.00 | 16.14 |
| ATOM | 3583 | C    | GLY | 142 | 6.307 | 13.802 | 6.702  | 1.00 | 17.47 |
| ATOM | 3584 | O    | GLY | 142 | 5.665 | 14.520 | 7.469  | 1.00 | 18.32 |
| ATOM | 3585 | H    | GLY | 142 | 8.113 | 16.160 | 6.259  | 1.00 | 0.00  |
| ATOM | 3586 | N    | ASP | 143 | 6.272 | 12.475 | 6.735  | 1.00 | 18.35 |
| ATOM | 3587 | CA   | ASP | 143 | 5.479 | 11.720 | 7.690  | 1.00 | 19.12 |
| ATOM | 3588 | C    | ASP | 143 | 5.818 | 12.116 | 9.115  | 1.00 | 20.80 |
| ATOM | 3589 | O    | ASP | 143 | 6.978 | 12.380 | 9.446  | 1.00 | 20.56 |
| ATOM | 3590 | CB   | ASP | 143 | 5.728 | 10.217 | 7.527  | 1.00 | 19.03 |
| ATOM | 3591 | CG   | ASP | 143 | 5.233 | 9.673  | 6.201  | 1.00 | 18.70 |
| ATOM | 3592 | OD1  | ASP | 143 | 4.551 | 10.410 | 5.448  | 1.00 | 19.38 |
| ATOM | 3593 | OD2  | ASP | 143 | 5.529 | 8.493  | 5.920  | 1.00 | 18.75 |
| ATOM | 3594 | H    | ASP | 143 | 6.807 | 11.996 | 6.066  | 1.00 | 0.00  |
| ATOM | 3595 | N    | VAL | 144 | 4.800 | 12.108 | 9.964  | 1.00 | 22.30 |
| ATOM | 3596 | CA   | VAL | 144 | 4.951 | 12.473 | 11.358 | 1.00 | 23.24 |
| ATOM | 3597 | C    | VAL | 144 | 5.292 | 11.281 | 12.236 | 1.00 | 25.57 |
| ATOM | 3598 | O    | VAL | 144 | 5.557 | 11.442 | 13.426 | 1.00 | 26.10 |
| ATOM | 3599 | CB   | VAL | 144 | 3.688 | 13.143 | 11.871 | 1.00 | 21.79 |
| ATOM | 3600 | CG1  | VAL | 144 | 3.441 | 14.423 | 11.094 | 1.00 | 21.10 |
| ATOM | 3601 | CG2  | VAL | 144 | 2.509 | 12.201 | 11.737 | 1.00 | 20.47 |
| ATOM | 3602 | H    | VAL | 144 | 3.953 | 11.795 | 9.605  | 1.00 | 0.00  |
| ATOM | 3603 | N    | ASP | 145 | 5.271 | 10.095 | 11.642 | 1.00 | 29.19 |
| ATOM | 3604 | CA   | ASP | 145 | 5.590 | 8.841  | 12.325 | 1.00 | 34.16 |
| ATOM | 3605 | C    | ASP | 145 | 5.562 | 7.790  | 11.220 | 1.00 | 36.85 |
| ATOM | 3606 | O    | ASP | 145 | 5.097 | 8.076  | 10.114 | 1.00 | 38.94 |
| ATOM | 3607 | CB   | ASP | 145 | 4.536 | 8.513  | 13.391 | 1.00 | 36.58 |
| ATOM | 3608 | CG   | ASP | 145 | 5.024 | 7.493  | 14.421 | 1.00 | 39.98 |
| ATOM | 3609 | OD1  | ASP | 145 | 5.675 | 6.493  | 14.049 | 1.00 | 42.07 |
| ATOM | 3610 | OD2  | ASP | 145 | 4.760 | 7.691  | 15.624 | 1.00 | 41.75 |
| ATOM | 3611 | H    | ASP | 145 | 5.012 | 10.034 | 10.696 | 1.00 | 0.00  |
| ATOM | 3612 | N    | ASN | 146 | 6.102 | 6.604  | 11.484 | 1.00 | 37.99 |
| ATOM | 3613 | CA   | ASN | 146 | 6.112 | 5.531  | 10.493 | 1.00 | 40.65 |
| ATOM | 3614 | C    | ASN | 146 | 4.690 | 5.290  | 9.989  | 1.00 | 41.93 |
| ATOM | 3615 | O    | ASN | 146 | 3.798 | 4.951  | 10.769 | 1.00 | 42.73 |
| ATOM | 3616 | CB   | ASN | 146 | 6.684 | 4.241  | 11.099 | 1.00 | 42.59 |
| ATOM | 3617 | CG   | ASN | 146 | 8.114 | 4.405  | 11.593 | 1.00 | 44.98 |
| ATOM | 3618 | OD1  | ASN | 146 | 9.078 | 4.147  | 10.866 | 1.00 | 45.48 |
| ATOM | 3619 | ND2  | ASN | 146 | 8.256 | 4.858  | 12.832 | 1.00 | 46.50 |
| ATOM | 3620 | H    | ASN | 146 | 6.501 | 6.482  | 12.364 | 1.00 | 0.00  |
| ATOM | 3621 | HD21 | ASN | 146 | 7.433 | 5.081  | 13.338 | 1.00 | 0.00  |
| ATOM | 3622 | HD22 | ASN | 146 | 9.151 | 4.976  | 13.213 | 1.00 | 0.00  |
| ATOM | 3623 | N    | ASP | 147 | 4.483 | 5.516  | 8.695  | 1.00 | 42.89 |
| ATOM | 3624 | CA   | ASP | 147 | 3.182 | 5.348  | 8.051  | 1.00 | 43.77 |
| ATOM | 3625 | C    | ASP | 147 | 2.153 | 6.353  | 8.526  | 1.00 | 43.61 |
| ATOM | 3626 | O    | ASP | 147 | 0.952 | 6.112  | 8.441  | 1.00 | 45.41 |
| ATOM | 3627 | CB   | ASP | 147 | 2.635 | 3.929  | 8.236  | 1.00 | 46.19 |
| ATOM | 3628 | CG   | ASP | 147 | 3.266 | 2.935  | 7.290  | 1.00 | 49.04 |
| ATOM | 3629 | OD1  | ASP | 147 | 3.502 | 3.289  | 6.111  | 1.00 | 49.80 |
| ATOM | 3630 | OD2  | ASP | 147 | 3.528 | 1.793  | 7.727  | 1.00 | 50.69 |
| ATOM | 3631 | H    | ASP | 147 | 5.215 | 5.831  | 8.129  | 1.00 | 0.00  |
| ATOM | 3632 | N    | GLU | 149 | 2.619 | 7.489  | 9.017  | 1.00 | 42.94 |
| ATOM | 3633 | CA   | GLU | 149 | 1.723 | 8.527  | 9.485  | 1.00 | 43.32 |
| ATOM | 3634 | C    | GLU | 149 | 1.942 | 9.752  | 8.633  | 1.00 | 42.86 |

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|      |      |      |     |      |        |        |        |      |       |
|------|------|------|-----|------|--------|--------|--------|------|-------|
| ATOM | 3635 | O    | GLU | 149  | 2.821  | 10.557 | 8.924  | 1.00 | 43.45 |
| ATOM | 3636 | CB   | GLU | 149  | 2.005  | 8.859  | 10.942 | 1.00 | 45.78 |
| ATOM | 3637 | CG   | GLU | 149  | 1.350  | 7.925  | 11.931 | 1.00 | 50.19 |
| ATOM | 3638 | CD   | GLU | 149  | 0.491  | 8.671  | 12.933 | 1.00 | 52.83 |
| ATOM | 3639 | OE1  | GLU | 149  | -0.392 | 9.447  | 12.497 | 1.00 | 55.40 |
| ATOM | 3640 | OE2  | GLU | 149  | 0.695  | 8.488  | 14.153 | 1.00 | 54.00 |
| ATOM | 3641 | H    | GLU | 149  | 3.580  | 7.654  | 9.060  | 1.00 | 0.00  |
| ATOM | 3642 | N    | ARG | 150  | 1.172  | 9.876  | 7.559  | 1.00 | 41.94 |
| ATOM | 3643 | CA   | ARG | 150  | 1.294  | 11.020 | 6.663  | 1.00 | 41.29 |
| ATOM | 3644 | C    | ARG | 150  | 1.051  | 12.332 | 7.400  | 1.00 | 37.71 |
| ATOM | 3645 | O    | ARG | 150  | 0.392  | 12.358 | 8.443  | 1.00 | 37.36 |
| ATOM | 3646 | CB   | ARG | 150  | 0.284  | 10.927 | 5.514  | 1.00 | 45.83 |
| ATOM | 3647 | CG   | ARG | 150  | 0.716  | 10.127 | 4.294  | 1.00 | 51.41 |
| ATOM | 3648 | CD   | ARG | 150  | -0.297 | 10.305 | 3.142  | 1.00 | 56.94 |
| ATOM | 3649 | NE   | ARG | 150  | -0.309 | 11.664 | 2.578  | 1.00 | 61.35 |
| ATOM | 3650 | CZ   | ARG | 150  | -1.307 | 12.545 | 2.711  | 1.00 | 63.02 |
| ATOM | 3651 | NH1  | ARG | 150  | -2.406 | 12.229 | 3.396  | 1.00 | 63.70 |
| ATOM | 3652 | NH2  | ARG | 150  | -1.203 | 13.749 | 2.151  | 1.00 | 62.91 |
| ATOM | 3653 | H    | ARG | 150  | 0.511  | 9.174  | 7.402  | 1.00 | 0.00  |
| ATOM | 3654 | HE   | ARG | 150  | 0.500  | 11.913 | 2.079  | 1.00 | 0.00  |
| ATOM | 3655 | HH11 | ARG | 150  | -2.497 | 11.328 | 3.827  | 1.00 | 0.00  |
| ATOM | 3656 | HH12 | ARG | 150  | -3.179 | 12.853 | 3.521  | 1.00 | 0.00  |
| ATOM | 3657 | HH21 | ARG | 150  | -0.397 | 14.023 | 1.608  | 1.00 | 0.00  |
| ATOM | 3658 | HH22 | ARG | 150  | -1.919 | 14.441 | 2.229  | 1.00 | 0.00  |
| ATOM | 3659 | N    | LEU | 151  | 1.606  | 13.412 | 6.862  | 1.00 | 33.58 |
| ATOM | 3660 | CA   | LEU | 151  | 1.415  | 14.738 | 7.434  | 1.00 | 30.33 |
| ATOM | 3661 | C    | LEU | 151  | 0.016  | 15.146 | 6.998  | 1.00 | 29.75 |
| ATOM | 3662 | O    | LEU | 151  | -0.240 | 15.359 | 5.810  | 1.00 | 32.33 |
| ATOM | 3663 | CB   | LEU | 151  | 2.438  | 15.718 | 6.857  | 1.00 | 29.57 |
| ATOM | 3664 | CG   | LEU | 151  | 2.288  | 17.196 | 7.227  | 1.00 | 28.37 |
| ATOM | 3665 | CD1  | LEU | 151  | 2.698  | 17.417 | 8.671  | 1.00 | 27.54 |
| ATOM | 3666 | CD2  | LEU | 151  | 3.136  | 18.049 | 6.295  | 1.00 | 27.57 |
| ATOM | 3667 | H    | LEU | 151  | 2.183  | 13.304 | 6.079  | 1.00 | 0.00  |
| ATOM | 3668 | N    | PRO | 152  | -0.920 | 15.231 | 7.942  | 1.00 | 27.48 |
| ATOM | 3669 | CA   | PRO | 152  | -2.289 | 15.612 | 7.600  | 1.00 | 25.97 |
| ATOM | 3670 | C    | PRO | 152  | -2.425 | 17.049 | 7.100  | 1.00 | 24.76 |
| ATOM | 3671 | O    | PRO | 152  | -1.610 | 17.920 | 7.428  | 1.00 | 25.13 |
| ATOM | 3672 | CB   | PRO | 152  | -3.017 | 15.430 | 8.925  | 1.00 | 26.39 |
| ATOM | 3673 | CG   | PRO | 152  | -1.977 | 15.825 | 9.910  | 1.00 | 27.66 |
| ATOM | 3674 | CD   | PRO | 152  | -0.765 | 15.087 | 9.397  | 1.00 | 27.22 |
| ATOM | 3675 | N    | PRO | 152A | -3.424 | 17.304 | 6.240  | 1.00 | 22.89 |
| ATOM | 3676 | CA   | PRO | 152A | -3.642 | 18.656 | 5.717  | 1.00 | 21.45 |
| ATOM | 3677 | C    | PRO | 152A | -4.019 | 19.579 | 6.878  | 1.00 | 20.40 |
| ATOM | 3678 | O    | PRO | 152A | -4.628 | 19.136 | 7.848  | 1.00 | 21.48 |
| ATOM | 3679 | CB   | PRO | 152A | -4.802 | 18.457 | 4.740  | 1.00 | 20.23 |
| ATOM | 3680 | CG   | PRO | 152A | -5.485 | 17.221 | 5.235  | 1.00 | 20.11 |
| ATOM | 3681 | CD   | PRO | 152A | -4.342 | 16.343 | 5.610  | 1.00 | 21.47 |
| ATOM | 3682 | N    | PRO | 152B | -3.627 | 20.861 | 6.822  | 1.00 | 19.54 |
| ATOM | 3683 | CA   | PRO | 152B | -3.130 | 21.633 | 5.682  | 1.00 | 20.04 |
| ATOM | 3684 | C    | PRO | 152B | -1.614 | 21.535 | 5.424  | 1.00 | 20.39 |
| ATOM | 3685 | O    | PRO | 152B | -0.980 | 22.533 | 5.054  | 1.00 | 20.71 |
| ATOM | 3686 | CB   | PRO | 152B | -3.534 | 23.053 | 6.059  | 1.00 | 19.55 |
| ATOM | 3687 | CG   | PRO | 152B | -3.275 | 23.066 | 7.514  | 1.00 | 17.27 |
| ATOM | 3688 | CD   | PRO | 152B | -3.874 | 21.753 | 7.969  | 1.00 | 18.19 |
| ATOM | 3689 | N    | PHE | 153  | -1.031 | 20.366 | 5.682  | 1.00 | 18.32 |
| ATOM | 3690 | CA   | PHE | 153  | 0.389  | 20.120 | 5.440  | 1.00 | 16.85 |
| ATOM | 3691 | C    | PHE | 153  | 1.321  | 21.248 | 5.902  | 1.00 | 17.00 |
| ATOM | 3692 | O    | PHE | 153  | 2.023  | 21.860 | 5.090  | 1.00 | 16.84 |
| ATOM | 3693 | CB   | PHE | 153  | 0.627  | 19.895 | 3.948  | 1.00 | 14.47 |
| ATOM | 3694 | CG   | PHE | 153  | -0.486 | 19.194 | 3.245  | 1.00 | 12.59 |
| ATOM | 3695 | CD1  | PHE | 153  | -1.423 | 19.921 | 2.521  | 1.00 | 11.93 |
| ATOM | 3696 | CD2  | PHE | 153  | -0.575 | 17.811 | 3.262  | 1.00 | 12.66 |
| ATOM | 3697 | CE1  | PHE | 153  | -2.429 | 19.281 | 1.819  | 1.00 | 11.58 |

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|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3698 | CE2  | PHE | 153 | -1.582 | 17.157 | 2.560  | 1.00 | 12.96 |
| ATOM | 3699 | CZ   | PHE | 153 | -2.511 | 17.893 | 1.836  | 1.00 | 12.43 |
| ATOM | 3700 | H    | PHE | 153 | -1.498 | 19.621 | 6.101  | 1.00 | 0.00  |
| ATOM | 3701 | N    | PRO | 154 | 1.349  | 21.535 | 7.205  | 1.00 | 16.98 |
| ATOM | 3702 | CA   | PRO | 154 | 2.224  | 22.607 | 7.685  | 1.00 | 18.46 |
| ATOM | 3703 | C    | PRO | 154 | 3.683  | 22.166 | 7.675  | 1.00 | 20.76 |
| ATOM | 3704 | O    | PRO | 154 | 3.964  | 20.976 | 7.796  | 1.00 | 23.06 |
| ATOM | 3705 | CB   | PRO | 154 | 1.728  | 22.814 | 9.106  | 1.00 | 18.11 |
| ATOM | 3706 | CG   | PRO | 154 | 1.398  | 21.404 | 9.538  | 1.00 | 17.22 |
| ATOM | 3707 | CD   | PRO | 154 | 0.690  | 20.838 | 8.325  | 1.00 | 17.21 |
| ATOM | 3708 | N    | LEU | 155 | 4.607  | 23.107 | 7.498  | 1.00 | 20.75 |
| ATOM | 3709 | CA   | LEU | 155 | 6.033  | 22.778 | 7.515  | 1.00 | 20.02 |
| ATOM | 3710 | C    | LEU | 155 | 6.431  | 22.537 | 8.969  | 1.00 | 20.39 |
| ATOM | 3711 | O    | LEU | 155 | 6.289  | 23.429 | 9.804  | 1.00 | 22.00 |
| ATOM | 3712 | CB   | LEU | 155 | 6.866  | 23.928 | 6.937  | 1.00 | 19.71 |
| ATOM | 3713 | CG   | LEU | 155 | 8.395  | 23.890 | 7.113  | 1.00 | 18.62 |
| ATOM | 3714 | CD1  | LEU | 155 | 8.985  | 22.667 | 6.439  | 1.00 | 18.68 |
| ATOM | 3715 | CD2  | LEU | 155 | 9.010  | 25.157 | 6.533  | 1.00 | 17.30 |
| ATOM | 3716 | H    | LEU | 155 | 4.308  | 24.025 | 7.345  | 1.00 | 0.00  |
| ATOM | 3717 | N    | LYS | 156 | 6.916  | 21.337 | 9.270  | 1.00 | 18.99 |
| ATOM | 3718 | CA   | LYS | 156 | 7.325  | 21.000 | 10.629 | 1.00 | 17.90 |
| ATOM | 3719 | C    | LYS | 156 | 8.836  | 21.054 | 10.807 | 1.00 | 17.45 |
| ATOM | 3720 | O    | LYS | 156 | 9.592  | 21.000 | 9.835  | 1.00 | 16.87 |
| ATOM | 3721 | CB   | LYS | 156 | 6.798  | 19.621 | 11.038 | 1.00 | 17.74 |
| ATOM | 3722 | CG   | LYS | 156 | 5.309  | 19.576 | 11.352 | 1.00 | 16.80 |
| ATOM | 3723 | CD   | LYS | 156 | 4.890  | 18.182 | 11.785 | 1.00 | 18.08 |
| ATOM | 3724 | CE   | LYS | 156 | 5.505  | 17.784 | 13.128 | 1.00 | 20.35 |
| ATOM | 3725 | NZ   | LYS | 156 | 5.344  | 16.329 | 13.460 | 1.00 | 20.97 |
| ATOM | 3726 | H    | LYS | 156 | 7.078  | 20.679 | 8.560  | 1.00 | 0.00  |
| ATOM | 3727 | HZ1  | LYS | 156 | 5.941  | 15.757 | 12.818 | 1.00 | 0.00  |
| ATOM | 3728 | HZ2  | LYS | 156 | 4.359  | 16.030 | 13.364 | 1.00 | 0.00  |
| ATOM | 3729 | HZ3  | LYS | 156 | 5.642  | 16.084 | 14.426 | 1.00 | 0.00  |
| ATOM | 3730 | N    | GLN | 157 | 9.258  | 21.123 | 12.067 | 1.00 | 18.39 |
| ATOM | 3731 | CA   | GLN | 157 | 10.664 | 21.210 | 12.450 | 1.00 | 19.27 |
| ATOM | 3732 | C    | GLN | 157 | 10.870 | 20.453 | 13.758 | 1.00 | 20.05 |
| ATOM | 3733 | O    | GLN | 157 | 9.923  | 20.256 | 14.517 | 1.00 | 20.91 |
| ATOM | 3734 | CB   | GLN | 157 | 11.018 | 22.675 | 12.712 | 1.00 | 19.96 |
| ATOM | 3735 | CG   | GLN | 157 | 10.229 | 23.272 | 13.895 | 1.00 | 19.36 |
| ATOM | 3736 | CD   | GLN | 157 | 10.516 | 24.742 | 14.160 | 1.00 | 20.05 |
| ATOM | 3737 | OE1  | GLN | 157 | 10.802 | 25.522 | 13.242 | 1.00 | 20.12 |
| ATOM | 3738 | NE2  | GLN | 157 | 10.418 | 25.132 | 15.420 | 1.00 | 19.86 |
| ATOM | 3739 | H    | GLN | 157 | 8.590  | 21.162 | 12.782 | 1.00 | 0.00  |
| ATOM | 3740 | HE21 | GLN | 157 | 10.162 | 24.470 | 16.090 | 1.00 | 0.00  |
| ATOM | 3741 | HE22 | GLN | 157 | 10.606 | 26.072 | 15.608 | 1.00 | 0.00  |
| ATOM | 3742 | N    | VAL | 158 | 12.110 | 20.076 | 14.044 | 1.00 | 19.79 |
| ATOM | 3743 | CA   | VAL | 158 | 12.424 | 19.388 | 15.286 | 1.00 | 19.85 |
| ATOM | 3744 | C    | VAL | 158 | 13.897 | 19.544 | 15.617 | 1.00 | 22.43 |
| ATOM | 3745 | O    | VAL | 158 | 14.737 | 19.550 | 14.716 | 1.00 | 24.62 |
| ATOM | 3746 | CB   | VAL | 158 | 12.078 | 17.898 | 15.224 | 1.00 | 18.99 |
| ATOM | 3747 | CG1  | VAL | 158 | 12.969 | 17.169 | 14.239 | 1.00 | 19.16 |
| ATOM | 3748 | CG2  | VAL | 158 | 12.218 | 17.303 | 16.587 | 1.00 | 20.14 |
| ATOM | 3749 | H    | VAL | 158 | 12.819 | 20.239 | 13.382 | 1.00 | 0.00  |
| ATOM | 3750 | N    | LYS | 159 | 14.206 | 19.729 | 16.896 | 1.00 | 24.32 |
| ATOM | 3751 | CA   | LYS | 159 | 15.596 | 19.870 | 17.318 | 1.00 | 26.22 |
| ATOM | 3752 | C    | LYS | 159 | 16.181 | 18.476 | 17.484 | 1.00 | 26.66 |
| ATOM | 3753 | O    | LYS | 159 | 15.661 | 17.669 | 18.256 | 1.00 | 27.72 |
| ATOM | 3754 | CB   | LYS | 159 | 15.702 | 20.640 | 18.640 | 1.00 | 28.05 |
| ATOM | 3755 | CG   | LYS | 159 | 17.143 | 20.892 | 19.093 | 1.00 | 30.96 |
| ATOM | 3756 | CD   | LYS | 159 | 17.236 | 21.509 | 20.494 | 1.00 | 33.80 |
| ATOM | 3757 | CE   | LYS | 159 | 16.838 | 22.992 | 20.539 | 1.00 | 35.50 |
| ATOM | 3758 | NZ   | LYS | 159 | 17.792 | 23.911 | 19.836 | 1.00 | 36.76 |
| ATOM | 3759 | H    | LYS | 159 | 13.474 | 19.763 | 17.547 | 1.00 | 0.00  |
| ATOM | 3760 | HZ1  | LYS | 159 | 17.817 | 23.689 | 18.819 | 1.00 | 0.00  |

|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3761 | H22  | LYS | 159 | 18.746 | 23.834 | 20.239 | 1.00 | 0.00  |
| ATOM | 3762 | H23  | LYS | 159 | 17.456 | 24.891 | 19.940 | 1.00 | 0.00  |
| ATOM | 3763 | N    | VAL | 160 | 17.252 | 18.192 | 16.756 | 1.00 | 25.77 |
| ATOM | 3764 | CA   | VAL | 160 | 17.894 | 16.890 | 16.820 | 1.00 | 25.19 |
| ATOM | 3765 | C    | VAL | 160 | 19.331 | 17.005 | 17.307 | 1.00 | 24.85 |
| ATOM | 3766 | O    | VAL | 160 | 20.053 | 17.922 | 16.917 | 1.00 | 24.58 |
| ATOM | 3767 | CB   | VAL | 160 | 17.892 | 16.190 | 15.441 | 1.00 | 25.80 |
| ATOM | 3768 | CG1  | VAL | 160 | 16.480 | 15.826 | 15.039 | 1.00 | 26.37 |
| ATOM | 3769 | CG2  | VAL | 160 | 18.531 | 17.086 | 14.391 | 1.00 | 24.77 |
| ATOM | 3770 | H    | VAL | 160 | 17.623 | 18.884 | 16.195 | 1.00 | 0.00  |
| ATOM | 3771 | N    | PRO | 161 | 19.736 | 16.116 | 18.230 | 1.00 | 24.60 |
| ATOM | 3772 | CA   | PRO | 161 | 21.093 | 16.101 | 18.783 | 1.00 | 23.63 |
| ATOM | 3773 | C    | PRO | 161 | 22.051 | 15.391 | 17.833 | 1.00 | 23.67 |
| ATOM | 3774 | O    | PRO | 161 | 21.764 | 14.277 | 17.407 | 1.00 | 23.91 |
| ATOM | 3775 | CB   | PRO | 161 | 20.911 | 15.303 | 20.071 | 1.00 | 23.61 |
| ATOM | 3776 | CG   | PRO | 161 | 19.834 | 14.326 | 19.709 | 1.00 | 21.45 |
| ATOM | 3777 | CD   | PRO | 161 | 18.854 | 15.205 | 18.989 | 1.00 | 23.62 |
| ATOM | 3778 | N    | ILE | 162 | 23.145 | 16.052 | 17.460 | 1.00 | 24.01 |
| ATOM | 3779 | CA   | ILE | 162 | 24.147 | 15.457 | 16.564 | 1.00 | 24.35 |
| ATOM | 3780 | C    | ILE | 162 | 24.814 | 14.283 | 17.270 | 1.00 | 26.36 |
| ATOM | 3781 | O    | ILE | 162 | 25.017 | 14.314 | 18.485 | 1.00 | 28.28 |
| ATOM | 3782 | CB   | ILE | 162 | 25.265 | 16.471 | 16.180 | 1.00 | 22.68 |
| ATOM | 3783 | CG1  | ILE | 162 | 24.772 | 17.459 | 15.128 | 1.00 | 22.47 |
| ATOM | 3784 | CG2  | ILE | 162 | 26.488 | 15.748 | 15.635 | 1.00 | 22.99 |
| ATOM | 3785 | H    | ILE | 162 | 23.295 | 16.977 | 17.753 | 1.00 | 0.00  |
| ATOM | 3786 | CD   | ILE | 162 | 24.562 | 16.840 | 13.773 | 1.00 | 23.92 |
| ATOM | 3787 | N    | MET | 163 | 25.171 | 13.259 | 16.508 | 1.00 | 26.92 |
| ATOM | 3788 | CA   | MET | 163 | 25.835 | 12.096 | 17.071 | 1.00 | 27.14 |
| ATOM | 3789 | C    | MET | 163 | 27.113 | 11.847 | 16.294 | 1.00 | 26.70 |
| ATOM | 3790 | O    | MET | 163 | 27.169 | 12.043 | 15.080 | 1.00 | 26.56 |
| ATOM | 3791 | CB   | MET | 163 | 24.935 | 10.863 | 17.018 | 1.00 | 28.49 |
| ATOM | 3792 | CG   | MET | 163 | 25.540 | 9.660  | 17.706 | 1.00 | 32.12 |
| ATOM | 3793 | SD   | MET | 163 | 24.403 | 8.288  | 17.898 | 1.00 | 35.49 |
| ATOM | 3794 | CE   | MET | 163 | 23.078 | 9.094  | 18.802 | 1.00 | 36.50 |
| ATOM | 3795 | H    | MET | 163 | 25.009 | 13.295 | 15.549 | 1.00 | 0.00  |
| ATOM | 3796 | N    | GLU | 164 | 28.147 | 11.441 | 17.016 | 1.00 | 26.10 |
| ATOM | 3797 | CA   | GLU | 164 | 29.447 | 11.168 | 16.437 | 1.00 | 25.57 |
| ATOM | 3798 | C    | GLU | 164 | 29.351 | 9.860  | 15.650 | 1.00 | 24.91 |
| ATOM | 3799 | O    | GLU | 164 | 28.704 | 8.910  | 16.101 | 1.00 | 24.54 |
| ATOM | 3800 | CB   | GLU | 164 | 30.464 | 11.078 | 17.574 | 1.00 | 26.32 |
| ATOM | 3801 | CG   | GLU | 164 | 31.889 | 11.396 | 17.193 | 1.00 | 27.94 |
| ATOM | 3802 | CD   | GLU | 164 | 32.647 | 10.184 | 16.731 | 1.00 | 29.60 |
| ATOM | 3803 | OE1  | GLU | 164 | 32.110 | 9.066  | 16.859 | 1.00 | 30.62 |
| ATOM | 3804 | OE2  | GLU | 164 | 33.787 | 10.340 | 16.245 | 1.00 | 31.23 |
| ATOM | 3805 | H    | GLU | 164 | 28.029 | 11.296 | 17.974 | 1.00 | 0.00  |
| ATOM | 3806 | N    | ASN | 165 | 29.965 | 9.826  | 14.467 | 1.00 | 24.44 |
| ATOM | 3807 | CA   | ASN | 165 | 29.936 | 8.643  | 13.598 | 1.00 | 23.80 |
| ATOM | 3808 | C    | ASN | 165 | 30.196 | 7.323  | 14.314 | 1.00 | 25.34 |
| ATOM | 3809 | O    | ASN | 165 | 29.352 | 6.441  | 14.297 | 1.00 | 24.57 |
| ATOM | 3810 | CB   | ASN | 165 | 30.925 | 8.779  | 12.427 | 1.00 | 21.73 |
| ATOM | 3811 | CG   | ASN | 165 | 30.386 | 9.630  | 11.280 | 1.00 | 19.60 |
| ATOM | 3812 | OD1  | ASN | 165 | 29.701 | 10.625 | 11.497 | 1.00 | 18.77 |
| ATOM | 3813 | ND2  | ASN | 165 | 30.725 | 9.255  | 10.056 | 1.00 | 17.38 |
| ATOM | 3814 | H    | ASN | 165 | 30.458 | 10.612 | 14.157 | 1.00 | 0.00  |
| ATOM | 3815 | HD21 | ASN | 165 | 31.292 | 8.468  | 9.911  | 1.00 | 0.00  |
| ATOM | 3816 | HD22 | ASN | 165 | 30.350 | 9.786  | 9.318  | 1.00 | 0.00  |
| ATOM | 3817 | N    | HIS | 166 | 31.339 | 7.210  | 14.985 | 1.00 | 29.08 |
| ATOM | 3818 | CA   | HIS | 166 | 31.720 | 5.981  | 15.690 | 1.00 | 31.78 |
| ATOM | 3819 | C    | HIS | 166 | 30.678 | 5.492  | 16.683 | 1.00 | 30.56 |
| ATOM | 3820 | O    | HIS | 166 | 30.415 | 4.291  | 16.779 | 1.00 | 29.97 |
| ATOM | 3821 | CB   | HIS | 166 | 33.062 | 6.161  | 16.396 | 1.00 | 37.52 |
| ATOM | 3822 | CG   | HIS | 166 | 34.184 | 6.513  | 15.470 | 1.00 | 44.81 |
| ATOM | 3823 | ND1  | HIS | 166 | 34.720 | 7.781  | 15.397 | 1.00 | 48.34 |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3824 | CD2 | HIS | 166 | 34.864 | 5.767  | 14.566 | 1.00 | 47.83 |
| ATOM | 3825 | CE1 | HIS | 166 | 35.678 | 7.805  | 14.487 | 1.00 | 50.35 |
| ATOM | 3826 | NE2 | HIS | 166 | 35.786 | 6.593  | 13.968 | 1.00 | 50.40 |
| ATOM | 3827 | H   | HIS | 166 | 31.909 | 8.003  | 15.080 | 1.00 | 0.00  |
| ATOM | 3828 | HD1 | HIS | 166 | 34.436 | 8.547  | 15.962 | 1.00 | 0.00  |
| ATOM | 3829 | HE2 | HIS | 166 | 36.430 | 6.307  | 13.297 | 1.00 | 0.00  |
| ATOM | 3830 | N   | ILE | 167 | 30.099 | 6.420  | 17.433 | 1.00 | 29.81 |
| ATOM | 3831 | CA  | ILE | 167 | 29.069 | 6.066  | 18.406 | 1.00 | 28.28 |
| ATOM | 3832 | C   | ILE | 167 | 27.817 | 5.604  | 17.659 | 1.00 | 28.58 |
| ATOM | 3833 | O   | ILE | 167 | 27.121 | 4.671  | 18.084 | 1.00 | 29.23 |
| ATOM | 3834 | CB  | ILE | 167 | 28.745 | 7.267  | 19.319 | 1.00 | 25.29 |
| ATOM | 3835 | CG1 | ILE | 167 | 29.918 | 7.516  | 20.263 | 1.00 | 22.49 |
| ATOM | 3836 | CG2 | ILE | 167 | 27.474 | 7.024  | 20.102 | 1.00 | 25.92 |
| ATOM | 3837 | H   | ILE | 167 | 30.420 | 7.343  | 17.333 | 1.00 | 0.00  |
| ATOM | 3838 | CD  | ILE | 167 | 30.225 | 6.346  | 21.150 | 1.00 | 19.13 |
| ATOM | 3839 | N   | CYS | 168 | 27.572 | 6.238  | 16.517 | 1.00 | 27.21 |
| ATOM | 3840 | CA  | CYS | 168 | 26.420 | 5.936  | 15.681 | 1.00 | 24.91 |
| ATOM | 3841 | C   | CYS | 168 | 26.536 | 4.595  | 14.978 | 1.00 | 23.89 |
| ATOM | 3842 | O   | CYS | 168 | 25.588 | 3.816  | 14.953 | 1.00 | 24.59 |
| ATOM | 3843 | CB  | CYS | 168 | 26.237 | 7.037  | 14.652 | 1.00 | 23.00 |
| ATOM | 3844 | SG  | CYS | 168 | 24.641 | 6.989  | 13.801 | 1.00 | 19.58 |
| ATOM | 3845 | H   | CYS | 168 | 28.172 | 6.967  | 16.256 | 1.00 | 0.00  |
| ATOM | 3846 | N   | ASP | 169 | 27.695 | 4.332  | 14.395 | 1.00 | 22.73 |
| ATOM | 3847 | CA  | ASP | 169 | 27.928 | 3.078  | 13.705 | 1.00 | 22.97 |
| ATOM | 3848 | C   | ASP | 169 | 27.700 | 1.939  | 14.700 | 1.00 | 23.84 |
| ATOM | 3849 | O   | ASP | 169 | 27.077 | 0.923  | 14.373 | 1.00 | 24.60 |
| ATOM | 3850 | CB  | ASP | 169 | 29.353 | 3.045  | 13.156 | 1.00 | 23.86 |
| ATOM | 3851 | CG  | ASP | 169 | 29.576 | 1.912  | 12.182 | 1.00 | 26.51 |
| ATOM | 3852 | OD1 | ASP | 169 | 28.592 | 1.453  | 11.569 | 1.00 | 27.87 |
| ATOM | 3853 | OD2 | ASP | 169 | 30.736 | 1.476  | 12.016 | 1.00 | 28.55 |
| ATOM | 3854 | H   | ASP | 169 | 28.392 | 4.986  | 14.412 | 1.00 | 0.00  |
| ATOM | 3855 | N   | ALA | 170 | 28.142 | 2.159  | 15.937 | 1.00 | 23.68 |
| ATOM | 3856 | CA  | ALA | 170 | 27.997 | 1.193  | 17.024 | 1.00 | 22.37 |
| ATOM | 3857 | C   | ALA | 170 | 26.545 | 0.776  | 17.184 | 1.00 | 20.80 |
| ATOM | 3858 | O   | ALA | 170 | 26.236 | -0.395 | 17.386 | 1.00 | 21.39 |
| ATOM | 3859 | CB  | ALA | 170 | 28.499 | 1.796  | 18.322 | 1.00 | 23.79 |
| ATOM | 3860 | H   | ALA | 170 | 28.622 | 2.995  | 16.114 | 1.00 | 0.00  |
| ATOM | 3861 | N   | LYS | 171 | 25.654 | 1.745  | 17.063 | 1.00 | 19.15 |
| ATOM | 3862 | CA  | LYS | 171 | 24.233 | 1.492  | 17.191 | 1.00 | 20.10 |
| ATOM | 3863 | C   | LYS | 171 | 23.716 | 0.607  | 16.055 | 1.00 | 19.94 |
| ATOM | 3864 | O   | LYS | 171 | 22.983 | -0.355 | 16.294 | 1.00 | 20.69 |
| ATOM | 3865 | CB  | LYS | 171 | 23.480 | 2.822  | 17.203 | 1.00 | 21.21 |
| ATOM | 3866 | CG  | LYS | 171 | 24.150 | 3.881  | 18.062 | 1.00 | 21.17 |
| ATOM | 3867 | CD  | LYS | 171 | 23.824 | 3.698  | 19.517 | 1.00 | 21.72 |
| ATOM | 3868 | CE  | LYS | 171 | 22.585 | 4.481  | 19.862 | 1.00 | 22.89 |
| ATOM | 3869 | NZ  | LYS | 171 | 22.867 | 5.945  | 19.819 | 1.00 | 23.93 |
| ATOM | 3870 | H   | LYS | 171 | 25.990 | 2.650  | 16.890 | 1.00 | 0.00  |
| ATOM | 3871 | HZ1 | LYS | 171 | 23.249 | 6.252  | 18.902 | 1.00 | 0.00  |
| ATOM | 3872 | HZ2 | LYS | 171 | 23.579 | 6.142  | 20.560 | 1.00 | 0.00  |
| ATOM | 3873 | HZ3 | LYS | 171 | 22.024 | 6.494  | 20.069 | 1.00 | 0.00  |
| ATOM | 3874 | N   | TYR | 172 | 24.122 | 0.908  | 14.825 | 1.00 | 19.08 |
| ATOM | 3875 | CA  | TYR | 172 | 23.658 | 0.135  | 13.678 | 1.00 | 19.28 |
| ATOM | 3876 | C   | TYR | 172 | 24.064 | -1.322 | 13.712 | 1.00 | 21.15 |
| ATOM | 3877 | O   | TYR | 172 | 23.418 | -2.172 | 13.092 | 1.00 | 22.03 |
| ATOM | 3878 | CB  | TYR | 172 | 24.045 | 0.797  | 12.358 | 1.00 | 17.33 |
| ATOM | 3879 | CG  | TYR | 172 | 23.017 | 1.813  | 11.915 | 1.00 | 16.92 |
| ATOM | 3880 | CD1 | TYR | 172 | 22.956 | 3.073  | 12.506 | 1.00 | 17.60 |
| ATOM | 3881 | CD2 | TYR | 172 | 22.078 | 1.505  | 10.935 | 1.00 | 16.62 |
| ATOM | 3882 | CE1 | TYR | 172 | 21.986 | 3.999  | 12.136 | 1.00 | 16.87 |
| ATOM | 3883 | CE2 | TYR | 172 | 21.109 | 2.423  | 10.560 | 1.00 | 17.13 |
| ATOM | 3884 | CZ  | TYR | 172 | 21.070 | 3.669  | 11.166 | 1.00 | 17.08 |
| ATOM | 3885 | OH  | TYR | 172 | 20.119 | 4.589  | 10.795 | 1.00 | 18.81 |
| ATOM | 3886 | H   | TYR | 172 | 24.723 | 1.676  | 14.705 | 1.00 | 0.00  |

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|      |      |     |     |      |        |         |        |      |       |
|------|------|-----|-----|------|--------|---------|--------|------|-------|
| ATOM | 3887 | HH  | TYR | 172  | 19.627 | 4.211   | 10.073 | 1.00 | 0.00  |
| ATOM | 3888 | N   | HIS | 173  | 25.137 | -1.617  | 14.432 | 1.00 | 21.59 |
| ATOM | 3889 | CA  | HIS | 173  | 25.570 | -2.996  | 14.573 | 1.00 | 22.42 |
| ATOM | 3890 | C   | HIS | 173  | 24.785 | -3.636  | 15.708 | 1.00 | 24.81 |
| ATOM | 3891 | O   | HIS | 173  | 24.507 | -4.838  | 15.684 | 1.00 | 25.91 |
| ATOM | 3892 | CB  | HIS | 173  | 27.062 | -3.061  | 14.859 | 1.00 | 20.46 |
| ATOM | 3893 | CG  | HIS | 173  | 27.899 | -2.671  | 13.691 | 1.00 | 18.20 |
| ATOM | 3894 | ND1 | HIS | 173  | 28.356 | -3.585  | 12.769 | 1.00 | 17.81 |
| ATOM | 3895 | CD2 | HIS | 173  | 28.323 | -1.458  | 13.267 | 1.00 | 18.07 |
| ATOM | 3896 | CE1 | HIS | 173  | 29.022 | -2.949  | 11.822 | 1.00 | 18.52 |
| ATOM | 3897 | NE2 | HIS | 173  | 29.019 | -1.659  | 12.102 | 1.00 | 18.15 |
| ATOM | 3898 | H   | HIS | 173  | 25.644 | -0.875  | 14.824 | 1.00 | 0.00  |
| ATOM | 3899 | HD1 | HIS | 173  | 28.234 | -4.564  | 12.830 | 1.00 | 0.00  |
| ATOM | 3900 | HE2 | HIS | 173  | 29.511 | -0.946  | 11.624 | 1.00 | 0.00  |
| ATOM | 3901 | N   | LEU | 173A | 24.384 | -2.813  | 16.674 | 1.00 | 26.04 |
| ATOM | 3902 | CA  | LEU | 173A | 23.630 | -3.273  | 17.832 | 1.00 | 27.52 |
| ATOM | 3903 | C   | LEU | 173A | 22.260 | -3.809  | 17.431 | 1.00 | 27.26 |
| ATOM | 3904 | O   | LEU | 173A | 21.342 | -3.044  | 17.133 | 1.00 | 28.04 |
| ATOM | 3905 | CB  | LEU | 173A | 23.485 | -2.137  | 18.845 | 1.00 | 31.03 |
| ATOM | 3906 | CG  | LEU | 173A | 23.502 | -2.536  | 20.326 | 1.00 | 34.64 |
| ATOM | 3907 | CD1 | LEU | 173A | 23.961 | -1.346  | 21.165 | 1.00 | 35.28 |
| ATOM | 3908 | CD2 | LEU | 173A | 22.132 | -3.068  | 20.791 | 1.00 | 36.09 |
| ATOM | 3909 | H   | LEU | 173A | 24.608 | -1.858  | 16.631 | 1.00 | 0.00  |
| ATOM | 3910 | N   | GLY | 173B | 22.139 | -5.132  | 17.416 | 1.00 | 26.76 |
| ATOM | 3911 | CA  | GLY | 173B | 20.891 | -5.769  | 17.046 | 1.00 | 26.34 |
| ATOM | 3912 | C   | GLY | 173B | 20.935 | -6.315  | 15.632 | 1.00 | 26.87 |
| ATOM | 3913 | O   | GLY | 173B | 19.925 | -6.783  | 15.107 | 1.00 | 27.77 |
| ATOM | 3914 | H   | GLY | 173B | 22.933 | -5.677  | 17.604 | 1.00 | 0.00  |
| ATOM | 3915 | N   | ALA | 173C | 22.116 | -6.301  | 15.028 | 1.00 | 26.46 |
| ATOM | 3916 | CA  | ALA | 173C | 22.281 | -6.777  | 13.666 | 1.00 | 27.18 |
| ATOM | 3917 | C   | ALA | 173C | 23.362 | -7.849  | 13.583 | 1.00 | 28.08 |
| ATOM | 3918 | O   | ALA | 173C | 24.112 | -8.057  | 14.534 | 1.00 | 30.04 |
| ATOM | 3919 | CB  | ALA | 173C | 22.623 | -5.605  | 12.760 | 1.00 | 27.71 |
| ATOM | 3920 | H   | ALA | 173C | 22.935 | -5.987  | 15.464 | 1.00 | 0.00  |
| ATOM | 3921 | N   | TYR | 173D | 23.430 | -8.536  | 12.447 | 1.00 | 27.96 |
| ATOM | 3922 | CA  | TYR | 173D | 24.422 | -9.588  | 12.237 | 1.00 | 27.77 |
| ATOM | 3923 | C   | TYR | 173D | 25.723 | -9.049  | 11.653 | 1.00 | 26.96 |
| ATOM | 3924 | O   | TYR | 173D | 26.773 | -9.680  | 11.772 | 1.00 | 27.21 |
| ATOM | 3925 | CB  | TYR | 173D | 23.893 | -10.641 | 11.271 | 1.00 | 28.74 |
| ATOM | 3926 | CG  | TYR | 173D | 22.621 | -11.335 | 11.681 | 1.00 | 29.41 |
| ATOM | 3927 | CD1 | TYR | 173D | 22.547 | -12.080 | 12.858 | 1.00 | 28.70 |
| ATOM | 3928 | CD2 | TYR | 173D | 21.513 | -11.320 | 10.839 | 1.00 | 30.22 |
| ATOM | 3929 | CE1 | TYR | 173D | 21.401 | -12.800 | 13.177 | 1.00 | 29.46 |
| ATOM | 3930 | CE2 | TYR | 173D | 20.372 | -12.033 | 11.146 | 1.00 | 30.97 |
| ATOM | 3931 | CZ  | TYR | 173D | 20.318 | -12.774 | 12.308 | 1.00 | 30.75 |
| ATOM | 3932 | OH  | TYR | 173D | 19.179 | -13.504 | 12.564 | 1.00 | 31.93 |
| ATOM | 3933 | H   | TYR | 173D | 22.783 | -8.335  | 11.755 | 1.00 | 0.00  |
| ATOM | 3934 | HH  | TYR | 173D | 18.654 | -13.419 | 11.758 | 1.00 | 0.00  |
| ATOM | 3935 | N   | THR | 173E | 25.636 | -7.921  | 10.962 | 1.00 | 25.61 |
| ATOM | 3936 | CA  | THR | 173E | 26.799 | -7.319  | 10.341 | 1.00 | 25.40 |
| ATOM | 3937 | C   | THR | 173E | 27.946 | -7.207  | 11.348 | 1.00 | 27.58 |
| ATOM | 3938 | O   | THR | 173E | 27.763 | -6.725  | 12.478 | 1.00 | 27.28 |
| ATOM | 3939 | CB  | THR | 173E | 26.460 | -5.925  | 9.785  | 1.00 | 24.02 |
| ATOM | 3940 | OG1 | THR | 173E | 25.111 | -5.917  | 9.302  | 1.00 | 22.74 |
| ATOM | 3941 | CG2 | THR | 173E | 27.385 | -5.580  | 8.636  | 1.00 | 23.23 |
| ATOM | 3942 | H   | THR | 173E | 24.793 | -7.438  | 10.874 | 1.00 | 0.00  |
| ATOM | 3943 | HG1 | THR | 173E | 25.140 | -6.441  | 8.492  | 1.00 | 0.00  |
| ATOM | 3944 | N   | GLY | 173F | 29.124 | -7.658  | 10.923 | 1.00 | 29.32 |
| ATOM | 3945 | CA  | GLY | 173F | 30.301 | -7.625  | 11.769 | 1.00 | 32.00 |
| ATOM | 3946 | C   | GLY | 173F | 30.678 | -6.217  | 12.172 | 1.00 | 34.76 |
| ATOM | 3947 | O   | GLY | 173F | 30.589 | -5.293  | 11.362 | 1.00 | 34.01 |
| ATOM | 3948 | H   | GLY | 173F | 29.171 | -7.992  | 10.009 | 1.00 | 0.00  |
| ATOM | 3949 | N   | ASP | 173G | 31.113 | -6.054  | 13.419 | 1.00 | 38.04 |

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|      |      |      |     |      |        |        |        |      |       |
|------|------|------|-----|------|--------|--------|--------|------|-------|
| ATOM | 3950 | CA   | ASP | 173G | 31.497 | -4.747 | 13.943 | 1.00 | 40.65 |
| ATOM | 3951 | C    | ASP | 173G | 32.578 | -4.036 | 13.145 | 1.00 | 42.04 |
| ATOM | 3952 | O    | ASP | 173G | 32.655 | -2.808 | 13.156 | 1.00 | 43.25 |
| ATOM | 3953 | CB   | ASP | 173G | 31.880 | -4.838 | 15.421 | 1.00 | 41.44 |
| ATOM | 3954 | CG   | ASP | 173G | 30.688 | -4.629 | 16.340 | 1.00 | 43.66 |
| ATOM | 3955 | OD1  | ASP | 173G | 30.336 | -3.458 | 16.608 | 1.00 | 45.53 |
| ATOM | 3956 | OD2  | ASP | 173G | 30.087 | -5.632 | 16.771 | 1.00 | 43.77 |
| ATOM | 3957 | H    | ASP | 173G | 31.140 | -6.813 | 14.038 | 1.00 | 0.00  |
| ATOM | 3958 | N    | ASP | 173H | 33.383 | -4.802 | 12.419 | 1.00 | 43.27 |
| ATOM | 3959 | CA   | ASP | 173H | 34.439 | -4.221 | 11.600 | 1.00 | 45.93 |
| ATOM | 3960 | C    | ASP | 173H | 33.929 | -3.784 | 10.229 | 1.00 | 44.70 |
| ATOM | 3961 | O    | ASP | 173H | 34.706 | -3.351 | 9.368  | 1.00 | 45.44 |
| ATOM | 3962 | CB   | ASP | 173H | 35.622 | -5.185 | 11.466 | 1.00 | 51.39 |
| ATOM | 3963 | CG   | ASP | 173H | 36.475 | -5.242 | 12.732 | 1.00 | 56.30 |
| ATOM | 3964 | OD1  | ASP | 173H | 36.854 | -6.363 | 13.144 | 1.00 | 58.77 |
| ATOM | 3965 | OD2  | ASP | 173H | 36.754 | -4.169 | 13.322 | 1.00 | 57.79 |
| ATOM | 3966 | H    | ASP | 173H | 33.315 | -5.771 | 12.465 | 1.00 | 0.00  |
| ATOM | 3967 | N    | VAL | 173I | 32.623 | -3.922 | 10.024 | 1.00 | 41.33 |
| ATOM | 3968 | CA   | VAL | 173I | 31.991 | -3.515 | 8.781  | 1.00 | 38.26 |
| ATOM | 3969 | C    | VAL | 173I | 31.484 | -2.117 | 9.052  | 1.00 | 36.58 |
| ATOM | 3970 | O    | VAL | 173I | 30.802 | -1.894 | 10.049 | 1.00 | 36.82 |
| ATOM | 3971 | CB   | VAL | 173I | 30.784 | -4.399 | 8.438  | 1.00 | 38.72 |
| ATOM | 3972 | CG1  | VAL | 173I | 30.134 | -3.921 | 7.136  | 1.00 | 37.56 |
| ATOM | 3973 | CG2  | VAL | 173I | 31.211 | -5.859 | 8.342  | 1.00 | 39.09 |
| ATOM | 3974 | H    | VAL | 173I | 32.052 | -4.278 | 10.721 | 1.00 | 0.00  |
| ATOM | 3975 | N    | ARG | 174  | 31.826 | -1.171 | 8.187  | 1.00 | 34.82 |
| ATOM | 3976 | CA   | ARG | 174  | 31.382 | 0.196  | 8.386  | 1.00 | 33.41 |
| ATOM | 3977 | C    | ARG | 174  | 30.022 | 0.457  | 7.749  | 1.00 | 31.34 |
| ATOM | 3978 | O    | ARG | 174  | 29.910 | 0.658  | 6.540  | 1.00 | 33.32 |
| ATOM | 3979 | CB   | ARG | 174  | 32.433 | 1.181  | 7.875  | 1.00 | 36.21 |
| ATOM | 3980 | CG   | ARG | 174  | 32.200 | 2.601  | 8.365  | 1.00 | 40.74 |
| ATOM | 3981 | CD   | ARG | 174  | 33.398 | 3.486  | 8.113  | 1.00 | 42.22 |
| ATOM | 3982 | NE   | ARG | 174  | 34.578 | 2.993  | 8.808  | 1.00 | 43.78 |
| ATOM | 3983 | CZ   | ARG | 174  | 35.822 | 3.218  | 8.405  | 1.00 | 45.52 |
| ATOM | 3984 | NH1  | ARG | 174  | 36.049 | 3.940  | 7.312  | 1.00 | 46.09 |
| ATOM | 3985 | NH2  | ARG | 174  | 36.839 | 2.731  | 9.100  | 1.00 | 46.37 |
| ATOM | 3986 | H    | ARG | 174  | 32.389 | -1.405 | 7.421  | 1.00 | 0.00  |
| ATOM | 3987 | HE   | ARG | 174  | 34.403 | 2.489  | 9.637  | 1.00 | 0.00  |
| ATOM | 3988 | HH11 | ARG | 174  | 35.333 | 4.398  | 6.771  | 1.00 | 0.00  |
| ATOM | 3989 | HH12 | ARG | 174  | 36.991 | 4.002  | 6.960  | 1.00 | 0.00  |
| ATOM | 3990 | HH21 | ARG | 174  | 36.726 | 2.149  | 9.911  | 1.00 | 0.00  |
| ATOM | 3991 | HH22 | ARG | 174  | 37.786 | 2.809  | 8.747  | 1.00 | 0.00  |
| ATOM | 3992 | N    | ILE | 175  | 28.986 | 0.444  | 8.576  | 1.00 | 28.47 |
| ATOM | 3993 | CA   | ILE | 175  | 27.628 | 0.675  | 8.115  | 1.00 | 26.99 |
| ATOM | 3994 | C    | ILE | 175  | 27.432 | 2.136  | 7.767  | 1.00 | 26.69 |
| ATOM | 3995 | O    | ILE | 175  | 27.010 | 2.460  | 6.654  | 1.00 | 26.41 |
| ATOM | 3996 | CB   | ILE | 175  | 26.615 | 0.244  | 9.176  | 1.00 | 27.22 |
| ATOM | 3997 | CG1  | ILE | 175  | 26.630 | -1.283 | 9.308  | 1.00 | 27.52 |
| ATOM | 3998 | CG2  | ILE | 175  | 25.235 | 0.756  | 8.823  | 1.00 | 27.90 |
| ATOM | 3999 | H    | ILE | 175  | 29.152 | 0.326  | 9.538  | 1.00 | 0.00  |
| ATOM | 4000 | CD   | ILE | 175  | 25.818 | -1.815 | 10.465 | 1.00 | 28.13 |
| ATOM | 4001 | N    | VAL | 176  | 27.705 | 3.017  | 8.725  | 1.00 | 27.11 |
| ATOM | 4002 | CA   | VAL | 176  | 27.581 | 4.449  | 8.478  | 1.00 | 27.74 |
| ATOM | 4003 | C    | VAL | 176  | 28.954 | 4.980  | 8.067  | 1.00 | 28.52 |
| ATOM | 4004 | O    | VAL | 176  | 29.867 | 5.113  | 8.884  | 1.00 | 28.13 |
| ATOM | 4005 | CB   | VAL | 176  | 26.986 | 5.214  | 9.688  | 1.00 | 26.10 |
| ATOM | 4006 | CG1  | VAL | 176  | 27.761 | 4.942  | 10.923 | 1.00 | 26.68 |
| ATOM | 4007 | CG2  | VAL | 176  | 26.959 | 6.700  | 9.407  | 1.00 | 26.65 |
| ATOM | 4008 | H    | VAL | 176  | 28.037 | 2.699  | 9.601  | 1.00 | 0.00  |
| ATOM | 4009 | N    | ARG | 177  | 29.100 | 5.205  | 6.764  | 1.00 | 29.65 |
| ATOM | 4010 | CA   | ARG | 177  | 30.343 | 5.679  | 6.158  | 1.00 | 30.11 |
| ATOM | 4011 | C    | ARG | 177  | 30.839 | 7.043  | 6.652  | 1.00 | 28.52 |
| ATOM | 4012 | O    | ARG | 177  | 30.132 | 7.776  | 7.348  | 1.00 | 26.59 |

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|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 4013 | CB   | ARG | 177 | 30.197 | 5.718  | 4.628  | 1.00 | 32.96 |
| ATOM | 4014 | CG   | ARG | 177 | 29.559 | 4.476  | 3.981  | 1.00 | 36.76 |
| ATOM | 4015 | CD   | ARG | 177 | 30.370 | 3.205  | 4.196  | 1.00 | 39.35 |
| ATOM | 4016 | NE   | ARG | 177 | 30.339 | 2.340  | 3.015  | 1.00 | 41.18 |
| ATOM | 4017 | CZ   | ARG | 177 | 29.588 | 1.247  | 2.890  | 1.00 | 42.10 |
| ATOM | 4018 | NH1  | ARG | 177 | 28.783 | 0.864  | 3.880  | 1.00 | 42.61 |
| ATOM | 4019 | NH2  | ARG | 177 | 29.664 | 0.519  | 1.781  | 1.00 | 41.14 |
| ATOM | 4020 | H    | ARG | 177 | 28.323 | 5.057  | 6.189  | 1.00 | 0.00  |
| ATOM | 4021 | HE   | ARG | 177 | 30.910 | 2.641  | 2.278  | 1.00 | 0.00  |
| ATOM | 4022 | HH11 | ARG | 177 | 28.752 | 1.384  | 4.738  | 1.00 | 0.00  |
| ATOM | 4023 | HH12 | ARG | 177 | 28.150 | 0.090  | 3.844  | 1.00 | 0.00  |
| ATOM | 4024 | HH21 | ARG | 177 | 30.254 | 0.754  | 1.003  | 1.00 | 0.00  |
| ATOM | 4025 | HH22 | ARG | 177 | 29.105 | -0.298 | 1.666  | 1.00 | 0.00  |
| ATOM | 4026 | N    | ASP | 178 | 32.045 | 7.401  | 6.224  | 1.00 | 29.05 |
| ATOM | 4027 | CA   | ASP | 178 | 32.662 | 8.664  | 6.612  | 1.00 | 29.02 |
| ATOM | 4028 | C    | ASP | 178 | 32.037 | 9.905  | 5.962  | 1.00 | 28.32 |
| ATOM | 4029 | O    | ASP | 178 | 32.301 | 11.031 | 6.386  | 1.00 | 30.20 |
| ATOM | 4030 | CB   | ASP | 178 | 34.177 | 8.609  | 6.375  | 1.00 | 29.37 |
| ATOM | 4031 | CG   | ASP | 178 | 34.867 | 7.587  | 7.271  | 1.00 | 31.13 |
| ATOM | 4032 | OD1  | ASP | 178 | 35.090 | 7.879  | 8.464  | 1.00 | 32.35 |
| ATOM | 4033 | OD2  | ASP | 178 | 35.183 | 6.474  | 6.799  | 1.00 | 31.08 |
| ATOM | 4034 | H    | ASP | 178 | 32.572 | 6.821  | 5.633  | 1.00 | 0.00  |
| ATOM | 4035 | N    | ASP | 179 | 31.199 | .707   | 4.950  | 1.00 | 26.25 |
| ATOM | 4036 | CA   | ASP | 179 | 30.536 | 10.831 | 4.297  | 1.00 | 23.43 |
| ATOM | 4037 | C    | ASP | 179 | 29.093 | 10.934 | 4.781  | 1.00 | 22.91 |
| ATOM | 4038 | O    | ASP | 179 | 28.242 | 11.553 | 4.143  | 1.00 | 24.05 |
| ATOM | 4039 | CB   | ASP | 179 | 30.612 | 10.734 | 2.763  | 1.00 | 21.79 |
| ATOM | 4040 | CG   | ASP | 179 | 29.903 | 9.520  | 2.201  | 1.00 | 19.83 |
| ATOM | 4041 | OD1  | ASP | 179 | 29.987 | 8.427  | 2.799  | 1.00 | 20.18 |
| ATOM | 4042 | OD2  | ASP | 179 | 29.277 | 9.654  | 1.132  | 1.00 | 18.73 |
| ATOM | 4043 | H    | ASP | 179 | 31.015 | 8.814  | 4.590  | 1.00 | 0.00  |
| ATOM | 4044 | N    | MET | 180 | 28.831 | 10.339 | 5.937  | 1.00 | 21.35 |
| ATOM | 4045 | CA   | MET | 180 | 27.508 | 10.380 | 6.536  | 1.00 | 19.41 |
| ATOM | 4046 | C    | MET | 180 | 27.647 | 11.076 | 7.879  | 1.00 | 19.51 |
| ATOM | 4047 | O    | MET | 180 | 28.761 | 11.262 | 8.380  | 1.00 | 19.99 |
| ATOM | 4048 | CB   | MET | 180 | 26.948 | 8.966  | 6.707  | 1.00 | 18.25 |
| ATOM | 4049 | CG   | MET | 180 | 26.689 | 8.260  | 5.384  | 1.00 | 16.80 |
| ATOM | 4050 | SD   | MET | 180 | 26.513 | 6.481  | 5.534  | 1.00 | 16.44 |
| ATOM | 4051 | CE   | MET | 180 | 26.539 | 6.033  | 3.830  | 1.00 | 15.90 |
| ATOM | 4052 | H    | MET | 180 | 29.530 | 9.850  | 6.408  | 1.00 | 0.00  |
| ATOM | 4053 | N    | LEU | 181 | 26.518 | 11.494 | 8.433  | 1.00 | 18.94 |
| ATOM | 4054 | CA   | LEU | 181 | 26.471 | 12.185 | 9.710  | 1.00 | 18.97 |
| ATOM | 4055 | C    | LEU | 181 | 25.213 | 11.684 | 10.410 | 1.00 | 21.06 |
| ATOM | 4056 | O    | LEU | 181 | 24.217 | 11.389 | 9.747  | 1.00 | 24.08 |
| ATOM | 4057 | CB   | LEU | 181 | 26.403 | 13.698 | 9.468  | 1.00 | 16.56 |
| ATOM | 4058 | CG   | LEU | 181 | 26.092 | 14.664 | 10.618 | 1.00 | 17.36 |
| ATOM | 4059 | CD1  | LEU | 181 | 26.623 | 16.030 | 10.261 | 1.00 | 15.96 |
| ATOM | 4060 | CD2  | LEU | 181 | 24.592 | 14.730 | 10.921 | 1.00 | 14.35 |
| ATOM | 4061 | H    | LEU | 181 | 25.674 | 11.336 | 7.960  | 1.00 | 0.00  |
| ATOM | 4062 | N    | CYS | 182 | 25.257 | 11.572 | 11.733 | 1.00 | 20.56 |
| ATOM | 4063 | CA   | CYS | 182 | 24.109 | 11.100 | 12.497 | 1.00 | 20.63 |
| ATOM | 4064 | C    | CYS | 182 | 23.497 | 12.158 | 13.389 | 1.00 | 23.21 |
| ATOM | 4065 | O    | CYS | 182 | 24.202 | 13.019 | 13.927 | 1.00 | 24.72 |
| ATOM | 4066 | CB   | CYS | 182 | 24.503 | 9.923  | 13.363 | 1.00 | 18.83 |
| ATOM | 4067 | SG   | CYS | 182 | 24.877 | 8.436  | 12.415 | 1.00 | 18.84 |
| ATOM | 4068 | H    | CYS | 182 | 26.065 | 11.822 | 12.229 | 1.00 | 0.00  |
| ATOM | 4069 | N    | ALA | 183 | 22.187 | 12.059 | 13.579 | 1.00 | 23.87 |
| ATOM | 4070 | CA   | ALA | 183 | 21.458 | 12.992 | 14.417 | 1.00 | 25.45 |
| ATOM | 4071 | C    | ALA | 183 | 20.085 | 12.423 | 14.722 | 1.00 | 27.64 |
| ATOM | 4072 | O    | ALA | 183 | 19.590 | 11.570 | 13.988 | 1.00 | 28.99 |
| ATOM | 4073 | CB   | ALA | 183 | 21.327 | 14.330 | 13.708 | 1.00 | 25.67 |
| ATOM | 4074 | H    | ALA | 183 | 21.682 | 11.364 | 13.096 | 1.00 | 0.00  |
| ATOM | 4075 | N    | GLY | 184 | 19.500 | 12.853 | 15.836 | 1.00 | 29.08 |

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|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 4076 | CA   | GLY | 184 | 18.174 | 12.392 | 16.204 | 1.00 | 30.66 |
| ATOM | 4077 | C    | GLY | 184 | 18.148 | 11.430 | 17.369 | 1.00 | 32.35 |
| ATOM | 4078 | O    | GLY | 184 | 19.138 | 11.293 | 18.091 | 1.00 | 32.85 |
| ATOM | 4079 | H    | GLY | 184 | 20.035 | 13.409 | 16.440 | 1.00 | 0.00  |
| ATOM | 4080 | N    | ASN | 185 | 16.990 | 10.806 | 17.576 | 1.00 | 34.24 |
| ATOM | 4081 | CA   | ASN | 185 | 16.773 | 9.830  | 18.645 | 1.00 | 36.16 |
| ATOM | 4082 | C    | ASN | 185 | 15.407 | 9.161  | 18.440 | 1.00 | 36.57 |
| ATOM | 4083 | O    | ASN | 185 | 14.945 | 9.056  | 17.308 | 1.00 | 37.28 |
| ATOM | 4084 | CB   | ASN | 185 | 16.874 | 10.496 | 20.029 | 1.00 | 37.81 |
| ATOM | 4085 | CG   | ASN | 185 | 15.803 | 11.557 | 20.269 | 1.00 | 40.23 |
| ATOM | 4086 | OD1  | ASN | 185 | 14.766 | 11.582 | 19.608 | 1.00 | 42.19 |
| ATOM | 4087 | ND2  | ASN | 185 | 16.040 | 12.420 | 21.248 | 1.00 | 41.19 |
| ATOM | 4088 | H    | ASN | 185 | 16.224 | 11.035 | 16.997 | 1.00 | 0.00  |
| ATOM | 4089 | HD21 | ASN | 185 | 16.882 | 12.315 | 21.737 | 1.00 | 0.00  |
| ATOM | 4090 | HD22 | ASN | 185 | 15.374 | 13.105 | 21.443 | 1.00 | 0.00  |
| ATOM | 4091 | N    | THR | 186 | 14.760 | 8.716  | 19.516 | 1.00 | 36.33 |
| ATOM | 4092 | CA   | THR | 186 | 13.454 | 8.063  | 19.410 | 1.00 | 36.28 |
| ATOM | 4093 | C    | THR | 186 | 12.253 | 9.006  | 19.414 | 1.00 | 36.80 |
| ATOM | 4094 | O    | THR | 186 | 11.146 | 8.602  | 19.070 | 1.00 | 37.63 |
| ATOM | 4095 | CB   | THR | 186 | 13.236 | 7.042  | 20.547 | 1.00 | 36.18 |
| ATOM | 4096 | OG1  | THR | 186 | 14.469 | 6.817  | 21.244 | 1.00 | 36.17 |
| ATOM | 4097 | CG2  | THR | 186 | 12.716 | 5.727  | 19.985 | 1.00 | 35.79 |
| ATOM | 4098 | H    | THR | 186 | 15.156 | 8.726  | 20.408 | 1.00 | 0.00  |
| ATOM | 4099 | HG1  | THR | 186 | 14.334 | 6.120  | 21.896 | 1.00 | 0.00  |
| ATOM | 4100 | N    | ARG | 187 | 12.445 | 10.238 | 19.859 | 1.00 | 37.73 |
| ATOM | 4101 | CA   | ARG | 187 | 11.343 | 11.190 | 19.909 | 1.00 | 39.50 |
| ATOM | 4102 | C    | ARG | 187 | 11.448 | 12.278 | 18.858 | 1.00 | 38.23 |
| ATOM | 4103 | O    | ARG | 187 | 10.611 | 13.175 | 18.807 | 1.00 | 39.79 |
| ATOM | 4104 | CB   | ARG | 187 | 11.247 | 11.836 | 21.289 | 1.00 | 44.38 |
| ATOM | 4105 | CG   | ARG | 187 | 10.908 | 10.875 | 22.405 | 1.00 | 50.95 |
| ATOM | 4106 | CD   | ARG | 187 | 10.734 | 11.613 | 23.723 | 1.00 | 56.59 |
| ATOM | 4107 | NE   | ARG | 187 | 10.395 | 10.698 | 24.811 | 1.00 | 62.33 |
| ATOM | 4108 | CZ   | ARG | 187 | 9.188  | 10.164 | 25.004 | 1.00 | 65.53 |
| ATOM | 4109 | NH1  | ARG | 187 | 8.182  | 10.453 | 24.180 | 1.00 | 67.23 |
| ATOM | 4110 | NH2  | ARG | 187 | 8.986  | 9.330  | 26.020 | 1.00 | 66.84 |
| ATOM | 4111 | H    | ARG | 187 | 13.336 | 10.509 | 20.136 | 1.00 | 0.00  |
| ATOM | 4112 | HE   | ARG | 187 | 11.140 | 10.504 | 25.428 | 1.00 | 0.00  |
| ATOM | 4113 | HH1  | ARG | 187 | 8.325  | 11.070 | 23.402 | 1.00 | 0.00  |
| ATOM | 4114 | HH2  | ARG | 187 | 7.264  | 10.070 | 24.301 | 1.00 | 0.00  |
| ATOM | 4115 | HH21 | ARG | 187 | 9.734  | 9.106  | 26.652 | 1.00 | 0.00  |
| ATOM | 4116 | HH22 | ARG | 187 | 8.092  | 8.918  | 26.234 | 1.00 | 0.00  |
| ATOM | 4117 | N    | ARG | 188 | 12.508 | 12.239 | 18.063 | 1.00 | 35.90 |
| ATOM | 4118 | CA   | ARG | 188 | 12.705 | 13.227 | 17.012 | 1.00 | 33.59 |
| ATOM | 4119 | C    | ARG | 188 | 13.601 | 12.674 | 15.932 | 1.00 | 29.51 |
| ATOM | 4120 | O    | ARG | 188 | 14.695 | 12.196 | 16.217 | 1.00 | 29.73 |
| ATOM | 4121 | CB   | ARG | 188 | 13.291 | 14.521 | 17.562 | 1.00 | 37.14 |
| ATOM | 4122 | CG   | ARG | 188 | 14.264 | 14.366 | 18.711 | 1.00 | 41.29 |
| ATOM | 4123 | CD   | ARG | 188 | 13.561 | 14.599 | 20.032 | 1.00 | 44.24 |
| ATOM | 4124 | NE   | ARG | 188 | 12.931 | 15.919 | 20.073 | 1.00 | 48.74 |
| ATOM | 4125 | CZ   | ARG | 188 | 13.539 | 17.033 | 20.477 | 1.00 | 50.43 |
| ATOM | 4126 | NH1  | ARG | 188 | 14.805 | 16.993 | 20.881 | 1.00 | 50.97 |
| ATOM | 4127 | NH2  | ARG | 188 | 12.882 | 18.189 | 20.471 | 1.00 | 51.40 |
| ATOM | 4128 | H    | ARG | 188 | 13.195 | 11.549 | 18.176 | 1.00 | 0.00  |
| ATOM | 4129 | HE   | ARG | 188 | 12.000 | 15.929 | 19.733 | 1.00 | 0.00  |
| ATOM | 4130 | HH1  | ARG | 188 | 15.304 | 16.127 | 20.841 | 1.00 | 0.00  |
| ATOM | 4131 | HH2  | ARG | 188 | 15.315 | 17.802 | 21.170 | 1.00 | 0.00  |
| ATOM | 4132 | HH21 | ARG | 188 | 11.934 | 18.196 | 20.138 | 1.00 | 0.00  |
| ATOM | 4133 | HH22 | ARG | 188 | 13.281 | 19.061 | 20.751 | 1.00 | 0.00  |
| ATOM | 4134 | N    | ASP | 189 | 13.131 | 12.753 | 14.695 | 1.00 | 25.65 |
| ATOM | 4135 | CA   | ASP | 189 | 13.862 | 12.234 | 13.553 | 1.00 | 22.81 |
| ATOM | 4136 | C    | ASP | 189 | 13.154 | 12.654 | 12.270 | 1.00 | 23.81 |
| ATOM | 4137 | O    | ASP | 189 | 12.023 | 13.155 | 12.304 | 1.00 | 23.21 |
| ATOM | 4138 | CB   | ASP | 189 | 13.887 | 10.708 | 13.647 | 1.00 | 20.08 |

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|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 4139 | CG   | ASP | 189 | 14.761 | 10.058 | 12.602 | 1.00 | 18.91 |
| ATOM | 4140 | OD1  | ASP | 189 | 15.611 | 10.723 | 11.986 | 1.00 | 20.62 |
| ATOM | 4141 | OD2  | ASP | 189 | 14.614 | 8.844  | 12.416 | 1.00 | 19.86 |
| ATOM | 4142 | H    | ASP | 189 | 12.252 | 13.168 | 14.556 | 1.00 | 0.00  |
| ATOM | 4143 | N    | SER | 190 | 13.857 | 12.516 | 11.150 | 1.00 | 24.35 |
| ATOM | 4144 | CA   | SER | 190 | 13.320 | 12.828 | 9.838  | 1.00 | 23.42 |
| ATOM | 4145 | C    | SER | 190 | 12.369 | 11.686 | 9.491  | 1.00 | 22.61 |
| ATOM | 4146 | O    | SER | 190 | 12.163 | 10.771 | 10.287 | 1.00 | 23.32 |
| ATOM | 4147 | CB   | SER | 190 | 14.453 | 12.866 | 8.813  | 1.00 | 24.97 |
| ATOM | 4148 | OG   | SER | 190 | 15.566 | 13.603 | 9.286  | 1.00 | 28.00 |
| ATOM | 4149 | H    | SER | 190 | 14.782 | 12.210 | 11.188 | 1.00 | 0.00  |
| ATOM | 4150 | HG   | SER | 190 | 15.281 | 14.447 | 9.652  | 1.00 | 0.00  |
| ATOM | 4151 | N    | CYS | 191 | 11.822 | 11.701 | 8.288  | 1.00 | 21.46 |
| ATOM | 4152 | CA   | CYS | 191 | 10.915 | 10.647 | 7.905  | 1.00 | 20.84 |
| ATOM | 4153 | C    | CYS | 191 | 10.715 | 10.635 | 6.393  | 1.00 | 22.39 |
| ATOM | 4154 | O    | CYS | 191 | 11.327 | 11.428 | 5.678  | 1.00 | 22.92 |
| ATOM | 4155 | CB   | CYS | 191 | 9.602  | 10.850 | 8.643  | 1.00 | 20.34 |
| ATOM | 4156 | SG   | CYS | 191 | 8.767  | 9.295  | 9.032  | 1.00 | 21.01 |
| ATOM | 4157 | H    | CYS | 191 | 11.946 | 12.453 | 7.666  | 1.00 | 0.00  |
| ATOM | 4158 | N    | GLN | 192 | 9.885  | 9.723  | 5.894  | 1.00 | 23.45 |
| ATOM | 4159 | CA   | GLN | 192 | 9.636  | 9.632  | 4.455  | 1.00 | 23.39 |
| ATOM | 4160 | C    | GLN | 192 | 9.078  | 10.970 | 3.979  | 1.00 | 21.24 |
| ATOM | 4161 | O    | GLN | 192 | 8.166  | 11.515 | 4.584  | 1.00 | 21.78 |
| ATOM | 4162 | CB   | GLN | 192 | 8.642  | 8.506  | 4.147  | 1.00 | 26.70 |
| ATOM | 4163 | CG   | GLN | 192 | 8.939  | 7.167  | 4.837  | 1.00 | 32.08 |
| ATOM | 4164 | CD   | GLN | 192 | 10.274 | 6.551  | 4.427  | 1.00 | 35.71 |
| ATOM | 4165 | OE1  | GLN | 192 | 10.975 | 5.943  | 5.247  | 1.00 | 37.07 |
| ATOM | 4166 | NE2  | GLN | 192 | 10.628 | 6.696  | 3.150  | 1.00 | 36.78 |
| ATOM | 4167 | H    | GLN | 192 | 9.409  | 9.130  | 6.517  | 1.00 | 0.00  |
| ATOM | 4168 | HE21 | GLN | 192 | 10.052 | 7.165  | 2.521  | 1.00 | 0.00  |
| ATOM | 4169 | HE22 | GLN | 192 | 11.495 | 6.295  | 2.921  | 1.00 | 0.00  |
| ATOM | 4170 | N    | GLY | 193 | 9.650  | 11.520 | 2.920  | 1.00 | 20.25 |
| ATOM | 4171 | CA   | GLY | 193 | 9.169  | 12.796 | 2.428  | 1.00 | 20.12 |
| ATOM | 4172 | C    | GLY | 193 | 10.047 | 13.950 | 2.873  | 1.00 | 20.12 |
| ATOM | 4173 | O    | GLY | 193 | 9.924  | 15.068 | 2.348  | 1.00 | 21.70 |
| ATOM | 4174 | H    | GLY | 193 | 10.397 | 11.087 | 2.481  | 1.00 | 0.00  |
| ATOM | 4175 | N    | ASP | 194 | 10.887 | 13.698 | 3.874  | 1.00 | 18.41 |
| ATOM | 4176 | CA   | ASP | 194 | 11.816 | 14.701 | 4.380  | 1.00 | 16.56 |
| ATOM | 4177 | C    | ASP | 194 | 13.115 | 14.614 | 3.592  | 1.00 | 16.44 |
| ATOM | 4178 | O    | ASP | 194 | 13.831 | 15.599 | 3.475  | 1.00 | 16.99 |
| ATOM | 4179 | CB   | ASP | 194 | 12.120 | 14.479 | 5.864  | 1.00 | 15.81 |
| ATOM | 4180 | CG   | ASP | 194 | 10.983 | 14.907 | 6.775  | 1.00 | 15.83 |
| ATOM | 4181 | OD1  | ASP | 194 | 10.415 | 16.000 | 6.579  | 1.00 | 16.34 |
| ATOM | 4182 | OD2  | ASP | 194 | 10.670 | 14.152 | 7.715  | 1.00 | 16.46 |
| ATOM | 4183 | H    | ASP | 194 | 10.913 | 12.837 | 4.333  | 1.00 | 0.00  |
| ATOM | 4184 | N    | SER | 195 | 13.425 | 13.422 | 3.080  | 1.00 | 16.86 |
| ATOM | 4185 | CA   | SER | 195 | 14.634 | 13.170 | 2.299  | 1.00 | 16.92 |
| ATOM | 4186 | C    | SER | 195 | 14.981 | 14.332 | 1.407  | 1.00 | 17.31 |
| ATOM | 4187 | O    | SER | 195 | 14.110 | 14.889 | 0.752  | 1.00 | 17.68 |
| ATOM | 4188 | CB   | SER | 195 | 14.471 | 11.926 | 1.438  | 1.00 | 19.23 |
| ATOM | 4189 | OG   | SER | 195 | 14.661 | 10.742 | 2.196  | 1.00 | 20.26 |
| ATOM | 4190 | H    | SER | 195 | 12.817 | 12.703 | 3.288  | 1.00 | 0.00  |
| ATOM | 4191 | N    | GLY | 196 | 16.259 | 14.695 | 1.398  | 1.00 | 19.31 |
| ATOM | 4192 | CA   | GLY | 196 | 16.727 | 15.818 | 0.602  | 1.00 | 19.48 |
| ATOM | 4193 | C    | GLY | 196 | 16.723 | 17.106 | 1.406  | 1.00 | 19.76 |
| ATOM | 4194 | O    | GLY | 196 | 17.452 | 18.045 | 1.089  | 1.00 | 21.35 |
| ATOM | 4195 | H    | GLY | 196 | 16.901 | 14.173 | 1.911  | 1.00 | 0.00  |
| ATOM | 4196 | N    | GLY | 197 | 15.944 | 17.117 | 2.486  | 1.00 | 19.10 |
| ATOM | 4197 | CA   | GLY | 197 | 15.816 | 18.286 | 3.340  | 1.00 | 18.62 |
| ATOM | 4198 | C    | GLY | 197 | 17.076 | 18.701 | 4.064  | 1.00 | 18.16 |
| ATOM | 4199 | O    | GLY | 197 | 17.993 | 17.891 | 4.219  | 1.00 | 20.19 |
| ATOM | 4200 | H    | GLY | 197 | 15.409 | 16.346 | 2.744  | 1.00 | 0.00  |
| ATOM | 4201 | N    | PRO | 198 | 17.132 | 19.947 | 4.562  | 1.00 | 16.00 |

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|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 4202 | CA   | PRO | 198 | 18.304 | 20.452 | 5.269  | 1.00 | 15.35 |
| ATOM | 4203 | C    | PRO | 198 | 18.377 | 20.157 | 6.760  | 1.00 | 16.57 |
| ATOM | 4204 | O    | PRO | 198 | 17.356 | 19.989 | 7.435  | 1.00 | 15.77 |
| ATOM | 4205 | CB   | PRO | 198 | 18.203 | 21.951 | 5.028  | 1.00 | 13.89 |
| ATOM | 4206 | CG   | PRO | 198 | 16.739 | 22.179 | 5.159  | 1.00 | 13.54 |
| ATOM | 4207 | CD   | PRO | 198 | 16.146 | 21.026 | 4.363  | 1.00 | 15.18 |
| ATOM | 4208 | N    | LEU | 199 | 19.617 | 20.050 | 7.236  | 1.00 | 18.13 |
| ATOM | 4209 | CA   | LEU | 199 | 19.940 | 19.855 | 8.645  | 1.00 | 17.52 |
| ATOM | 4210 | C    | LEU | 199 | 20.842 | 21.056 | 8.875  | 1.00 | 17.54 |
| ATOM | 4211 | O    | LEU | 199 | 21.989 | 21.069 | 8.439  | 1.00 | 17.18 |
| ATOM | 4212 | CB   | LEU | 199 | 20.742 | 18.570 | 8.892  | 1.00 | 16.40 |
| ATOM | 4213 | CG   | LEU | 199 | 21.263 | 18.397 | 10.332 | 1.00 | 15.93 |
| ATOM | 4214 | CD1  | LEU | 199 | 20.118 | 18.054 | 11.261 | 1.00 | 16.34 |
| ATOM | 4215 | CD2  | LEU | 199 | 22.320 | 17.317 | 10.421 | 1.00 | 15.15 |
| ATOM | 4216 | H    | LEU | 199 | 20.367 | 20.071 | 6.609  | 1.00 | 0.00  |
| ATOM | 4217 | N    | VAL | 200 | 20.289 | 22.103 | 9.461  | 1.00 | 18.07 |
| ATOM | 4218 | CA   | VAL | 200 | 21.065 | 23.297 | 9.714  | 1.00 | 20.40 |
| ATOM | 4219 | C    | VAL | 200 | 21.463 | 23.352 | 11.173 | 1.00 | 23.18 |
| ATOM | 4220 | O    | VAL | 200 | 20.731 | 22.868 | 12.032 | 1.00 | 24.65 |
| ATOM | 4221 | CB   | VAL | 200 | 20.263 | 24.556 | 9.379  | 1.00 | 20.22 |
| ATOM | 4222 | CG1  | VAL | 200 | 20.014 | 24.629 | 7.891  | 1.00 | 20.48 |
| ATOM | 4223 | CG2  | VAL | 200 | 18.952 | 24.552 | 10.136 | 1.00 | 20.54 |
| ATOM | 4224 | H    | VAL | 200 | 19.381 | 21.997 | 9.815  | 1.00 | 0.00  |
| ATOM | 4225 | N    | CYS | 201 | 22.642 | 23.901 | 11.440 | 1.00 | 25.85 |
| ATOM | 4226 | CA   | CYS | 201 | 23.136 | 24.055 | 12.802 | 1.00 | 28.81 |
| ATOM | 4227 | C    | CYS | 201 | 23.606 | 25.503 | 12.958 | 1.00 | 32.04 |
| ATOM | 4228 | O    | CYS | 201 | 24.201 | 26.076 | 12.033 | 1.00 | 31.12 |
| ATOM | 4229 | CB   | CYS | 201 | 24.296 | 23.101 | 13.078 | 1.00 | 27.50 |
| ATOM | 4230 | SG   | CYS | 201 | 23.991 | 21.365 | 12.642 | 1.00 | 28.45 |
| ATOM | 4231 | H    | CYS | 201 | 23.184 | 24.212 | 10.689 | 1.00 | 0.00  |
| ATOM | 4232 | N    | LYS | 202 | 23.315 | 26.102 | 14.109 | 1.00 | 36.39 |
| ATOM | 4233 | CA   | LYS | 202 | 23.703 | 27.486 | 14.366 | 1.00 | 40.44 |
| ATOM | 4234 | C    | LYS | 202 | 25.145 | 27.570 | 14.860 | 1.00 | 42.60 |
| ATOM | 4235 | O    | LYS | 202 | 25.418 | 27.316 | 16.034 | 1.00 | 44.17 |
| ATOM | 4236 | CB   | LYS | 202 | 22.754 | 28.125 | 15.387 | 1.00 | 41.49 |
| ATOM | 4237 | CG   | LYS | 202 | 22.830 | 29.646 | 15.459 | 1.00 | 42.16 |
| ATOM | 4238 | CD   | LYS | 202 | 21.684 | 30.197 | 16.293 | 1.00 | 43.06 |
| ATOM | 4239 | CE   | LYS | 202 | 21.756 | 31.713 | 16.455 | 1.00 | 43.50 |
| ATOM | 4240 | NZ   | LYS | 202 | 21.441 | 32.499 | 15.227 | 1.00 | 42.33 |
| ATOM | 4241 | H    | LYS | 202 | 22.862 | 25.604 | 14.820 | 1.00 | 0.00  |
| ATOM | 4242 | HZ1  | LYS | 202 | 20.477 | 32.317 | 14.896 | 1.00 | 0.00  |
| ATOM | 4243 | HZ2  | LYS | 202 | 22.103 | 32.342 | 14.439 | 1.00 | 0.00  |
| ATOM | 4244 | HZ3  | LYS | 202 | 21.533 | 33.510 | 15.496 | 1.00 | 0.00  |
| ATOM | 4245 | N    | VAL | 203 | 26.063 | 27.905 | 13.960 | 1.00 | 43.88 |
| ATOM | 4246 | CA   | VAL | 203 | 27.476 | 28.023 | 14.302 | 1.00 | 45.25 |
| ATOM | 4247 | C    | VAL | 203 | 27.858 | 29.496 | 14.406 | 1.00 | 46.24 |
| ATOM | 4248 | O    | VAL | 203 | 27.961 | 30.196 | 13.393 | 1.00 | 47.09 |
| ATOM | 4249 | CB   | VAL | 203 | 28.364 | 27.306 | 13.257 | 1.00 | 45.79 |
| ATOM | 4250 | CG1  | VAL | 203 | 29.827 | 27.675 | 13.441 | 1.00 | 46.99 |
| ATOM | 4251 | CG2  | VAL | 203 | 28.202 | 25.803 | 13.391 | 1.00 | 47.34 |
| ATOM | 4252 | H    | VAL | 203 | 25.766 | 28.123 | 13.055 | 1.00 | 0.00  |
| ATOM | 4253 | N    | ASN | 204 | 28.044 | 29.960 | 15.640 | 1.00 | 46.28 |
| ATOM | 4254 | CA   | ASN | 204 | 28.400 | 31.350 | 15.902 | 1.00 | 46.85 |
| ATOM | 4255 | C    | ASN | 204 | 27.378 | 32.287 | 15.284 | 1.00 | 46.73 |
| ATOM | 4256 | O    | ASN | 204 | 27.703 | 33.094 | 14.415 | 1.00 | 47.28 |
| ATOM | 4257 | CB   | ASN | 204 | 29.794 | 31.669 | 15.354 | 1.00 | 49.65 |
| ATOM | 4258 | CG   | ASN | 204 | 30.892 | 31.016 | 16.156 | 1.00 | 52.80 |
| ATOM | 4259 | OD1  | ASN | 204 | 30.665 | 30.572 | 17.280 | 1.00 | 55.04 |
| ATOM | 4260 | ND2  | ASN | 204 | 32.092 | 30.946 | 15.586 | 1.00 | 53.78 |
| ATOM | 4261 | H    | ASN | 204 | 27.947 | 29.339 | 16.389 | 1.00 | 0.00  |
| ATOM | 4262 | HD21 | ASN | 204 | 32.202 | 31.311 | 14.686 | 1.00 | 0.00  |
| ATOM | 4263 | HD22 | ASN | 204 | 32.806 | 30.530 | 16.108 | 1.00 | 0.00  |
| ATOM | 4264 | N    | GLY | 205 | 26.122 | 32.127 | 15.686 | 1.00 | 45.97 |

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|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 4265 | CA   | GLY | 205 | 25.067 | 32.979 | 15.169 | 1.00 | 44.30 |
| ATOM | 4266 | C    | GLY | 205 | 24.561 | 32.676 | 13.769 | 1.00 | 43.64 |
| ATOM | 4267 | O    | GLY | 205 | 23.394 | 32.956 | 13.476 | 1.00 | 44.87 |
| ATOM | 4268 | H    | GLY | 205 | 25.926 | 31.422 | 16.335 | 1.00 | 0.00  |
| ATOM | 4269 | N    | THR | 206 | 25.399 | 32.075 | 12.927 | 1.00 | 41.35 |
| ATOM | 4270 | CA   | THR | 206 | 25.030 | 31.746 | 11.551 | 1.00 | 38.93 |
| ATOM | 4271 | C    | THR | 206 | 24.428 | 30.340 | 11.403 | 1.00 | 37.00 |
| ATOM | 4272 | O    | THR | 206 | 24.790 | 29.417 | 12.137 | 1.00 | 37.46 |
| ATOM | 4273 | CB   | THR | 206 | 26.270 | 31.870 | 10.637 | 1.00 | 38.86 |
| ATOM | 4274 | OG1  | THR | 206 | 26.847 | 33.167 | 10.810 | 1.00 | 39.45 |
| ATOM | 4275 | CG2  | THR | 206 | 25.900 | 31.703 | 9.180  | 1.00 | 39.45 |
| ATOM | 4276 | H    | THR | 206 | 26.322 | 31.854 | 13.177 | 1.00 | 0.00  |
| ATOM | 4277 | HG1  | THR | 206 | 27.742 | 33.163 | 10.462 | 1.00 | 0.00  |
| ATOM | 4278 | N    | TRP | 207 | 23.470 | 30.197 | 10.492 | 1.00 | 33.39 |
| ATOM | 4279 | CA   | TRP | 207 | 22.848 | 28.902 | 10.232 | 1.00 | 30.05 |
| ATOM | 4280 | C    | TRP | 207 | 23.559 | 28.240 | 9.065  | 1.00 | 29.13 |
| ATOM | 4281 | O    | TRP | 207 | 23.426 | 28.682 | 7.917  | 1.00 | 29.40 |
| ATOM | 4282 | CB   | TRP | 207 | 21.373 | 29.063 | 9.872  | 1.00 | 28.31 |
| ATOM | 4283 | CG   | TRP | 207 | 20.495 | 29.391 | 11.021 | 1.00 | 27.19 |
| ATOM | 4284 | CD1  | TRP | 207 | 19.933 | 30.598 | 11.299 | 1.00 | 27.65 |
| ATOM | 4285 | CD2  | TRP | 207 | 20.034 | 28.489 | 12.031 | 1.00 | 26.85 |
| ATOM | 4286 | NE1  | TRP | 207 | 19.143 | 30.505 | 12.418 | 1.00 | 27.40 |
| ATOM | 4287 | CE2  | TRP | 207 | 19.190 | 29.220 | 12.888 | 1.00 | 26.98 |
| ATOM | 4288 | CE3  | TRP | 207 | 20.251 | 27.130 | 12.294 | 1.00 | 27.81 |
| ATOM | 4289 | CZ2  | TRP | 207 | 18.560 | 28.641 | 13.993 | 1.00 | 27.99 |
| ATOM | 4290 | CZ3  | TRP | 207 | 19.626 | 26.551 | 13.389 | 1.00 | 26.42 |
| ATOM | 4291 | CH2  | TRP | 207 | 18.789 | 27.307 | 14.225 | 1.00 | 27.81 |
| ATOM | 4292 | H    | TRP | 207 | 23.170 | 30.965 | 9.966  | 1.00 | 0.00  |
| ATOM | 4293 | HE1  | TRP | 207 | 18.566 | 31.220 | 12.761 | 1.00 | 0.00  |
| ATOM | 4294 | N    | LEU | 208 | 24.317 | 27.191 | 9.356  | 1.00 | 28.79 |
| ATOM | 4295 | CA   | LEU | 208 | 25.049 | 26.460 | 8.322  | 1.00 | 28.46 |
| ATOM | 4296 | C    | LEU | 208 | 24.355 | 25.126 | 8.054  | 1.00 | 27.27 |
| ATOM | 4297 | O    | LEU | 208 | 23.770 | 24.538 | 8.967  | 1.00 | 27.37 |
| ATOM | 4298 | CB   | LEU | 208 | 26.479 | 26.183 | 8.783  | 1.00 | 28.49 |
| ATOM | 4299 | CG   | LEU | 208 | 27.330 | 27.363 | 9.236  | 1.00 | 28.03 |
| ATOM | 4300 | CD1  | LEU | 208 | 28.607 | 26.835 | 9.832  | 1.00 | 27.65 |
| ATOM | 4301 | CD2  | LEU | 208 | 27.623 | 28.280 | 8.064  | 1.00 | 28.25 |
| ATOM | 4302 | H    | LEU | 208 | 24.363 | 26.872 | 10.282 | 1.00 | 0.00  |
| ATOM | 4303 | N    | GLN | 209 | 24.412 | 24.641 | 6.816  | 1.00 | 24.85 |
| ATOM | 4304 | CA   | GLN | 209 | 23.782 | 23.363 | 6.525  | 1.00 | 23.01 |
| ATOM | 4305 | C    | GLN | 209 | 24.725 | 22.223 | 6.864  | 1.00 | 22.16 |
| ATOM | 4306 | O    | GLN | 209 | 25.691 | 21.968 | 6.149  | 1.00 | 21.33 |
| ATOM | 4307 | CB   | GLN | 209 | 23.328 | 23.256 | 5.074  | 1.00 | 22.73 |
| ATOM | 4308 | CG   | GLN | 209 | 22.667 | 21.912 | 4.789  | 1.00 | 22.97 |
| ATOM | 4309 | CD   | GLN | 209 | 21.673 | 21.954 | 3.649  | 1.00 | 22.55 |
| ATOM | 4310 | OE1  | GLN | 209 | 21.494 | 22.978 | 2.987  | 1.00 | 20.96 |
| ATOM | 4311 | NE2  | GLN | 209 | 20.998 | 20.838 | 3.432  | 1.00 | 23.79 |
| ATOM | 4312 | H    | GLN | 209 | 24.836 | 25.190 | 6.128  | 1.00 | 0.00  |
| ATOM | 4313 | HE21 | GLN | 209 | 21.180 | 20.072 | 4.017  | 1.00 | 0.00  |
| ATOM | 4314 | HE22 | GLN | 209 | 20.359 | 20.831 | 2.690  | 1.00 | 0.00  |
| ATOM | 4315 | N    | ALA | 210 | 24.443 | 21.565 | 7.982  | 1.00 | 21.93 |
| ATOM | 4316 | CA   | ALA | 210 | 25.237 | 20.450 | 8.467  | 1.00 | 22.31 |
| ATOM | 4317 | C    | ALA | 210 | 25.106 | 19.185 | 7.604  | 1.00 | 23.21 |
| ATOM | 4318 | O    | ALA | 210 | 26.094 | 18.481 | 7.383  | 1.00 | 23.35 |
| ATOM | 4319 | CB   | ALA | 210 | 24.868 | 20.152 | 9.914  | 1.00 | 21.07 |
| ATOM | 4320 | H    | ALA | 210 | 23.675 | 21.852 | 8.508  | 1.00 | 0.00  |
| ATOM | 4321 | N    | GLY | 211 | 23.904 | 18.909 | 7.101  | 1.00 | 22.83 |
| ATOM | 4322 | CA   | GLY | 211 | 23.701 | 17.716 | 6.289  | 1.00 | 20.07 |
| ATOM | 4323 | C    | GLY | 211 | 22.469 | 17.716 | 5.399  | 1.00 | 19.23 |
| ATOM | 4324 | O    | GLY | 211 | 21.763 | 18.727 | 5.283  | 1.00 | 19.11 |
| ATOM | 4325 | H    | GLY | 211 | 23.164 | 19.523 | 7.299  | 1.00 | 0.00  |
| ATOM | 4326 | N    | VAL | 212 | 22.235 | 16.577 | 4.751  | 1.00 | 18.04 |
| ATOM | 4327 | CA   | VAL | 212 | 21.101 | 16.378 | 3.844  | 1.00 | 16.65 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 4328 | C   | VAL | 212 | 20.419 | 15.061 | 4.237  | 1.00 | 16.31 |
| ATOM | 4329 | O   | VAL | 212 | 21.072 | 14.024 | 4.277  | 1.00 | 17.10 |
| ATOM | 4330 | CB  | VAL | 212 | 21.594 | 16.278 | 2.372  | 1.00 | 15.40 |
| ATOM | 4331 | CG1 | VAL | 212 | 20.449 | 15.937 | 1.433  | 1.00 | 14.08 |
| ATOM | 4332 | CG2 | VAL | 212 | 22.244 | 17.578 | 1.956  | 1.00 | 14.54 |
| ATOM | 4333 | H   | VAL | 212 | 22.869 | 15.846 | 4.878  | 1.00 | 0.00  |
| ATOM | 4334 | N   | VAL | 213 | 19.124 | 15.102 | 4.546  | 1.00 | 14.65 |
| ATOM | 4335 | CA  | VAL | 213 | 18.396 | 13.898 | 4.949  | 1.00 | 13.73 |
| ATOM | 4336 | C   | VAL | 213 | 18.564 | 12.817 | 3.883  | 1.00 | 14.82 |
| ATOM | 4337 | O   | VAL | 213 | 18.180 | 13.014 | 2.734  | 1.00 | 15.88 |
| ATOM | 4338 | CB  | VAL | 213 | 16.896 | 14.184 | 5.187  | 1.00 | 12.90 |
| ATOM | 4339 | CG1 | VAL | 213 | 16.255 | 13.004 | 5.882  | 1.00 | 11.62 |
| ATOM | 4340 | CG2 | VAL | 213 | 16.713 | 15.440 | 6.032  | 1.00 | 11.42 |
| ATOM | 4341 | H   | VAL | 213 | 18.684 | 15.976 | 4.484  | 1.00 | 0.00  |
| ATOM | 4342 | N   | SER | 214 | 19.139 | 11.682 | 4.271  | 1.00 | 16.75 |
| ATOM | 4343 | CA  | SER | 214 | 19.404 | 10.588 | 3.339  | 1.00 | 19.13 |
| ATOM | 4344 | C   | SER | 214 | 18.709 | 9.256  | 3.635  | 1.00 | 20.20 |
| ATOM | 4345 | O   | SER | 214 | 17.930 | 8.774  | 2.814  | 1.00 | 22.54 |
| ATOM | 4346 | CB  | SER | 214 | 20.925 | 10.384 | 3.203  | 1.00 | 19.61 |
| ATOM | 4347 | OG  | SER | 214 | 21.261 | 9.219  | 2.463  | 1.00 | 19.40 |
| ATOM | 4348 | H   | SER | 214 | 19.403 | 11.538 | 5.205  | 1.00 | 0.00  |
| ATOM | 4349 | HG  | SER | 214 | 21.080 | 9.374  | 1.529  | 1.00 | 0.00  |
| ATOM | 4350 | N   | TRP | 215 | 19.001 | 8.642  | 4.775  | 1.00 | 19.88 |
| ATOM | 4351 | CA  | TRP | 215 | 18.376 | 7.368  | 5.098  | 1.00 | 20.79 |
| ATOM | 4352 | C   | TRP | 215 | 18.356 | 7.020  | 6.584  | 1.00 | 22.87 |
| ATOM | 4353 | O   | TRP | 215 | 18.675 | 7.848  | 7.433  | 1.00 | 23.73 |
| ATOM | 4354 | CB  | TRP | 215 | 19.008 | 6.234  | 4.278  | 1.00 | 19.45 |
| ATOM | 4355 | CG  | TRP | 215 | 20.438 | 5.937  | 4.582  | 1.00 | 19.03 |
| ATOM | 4356 | CD1 | TRP | 215 | 21.526 | 6.653  | 4.182  | 1.00 | 19.67 |
| ATOM | 4357 | CD2 | TRP | 215 | 20.946 | 4.808  | 5.307  | 1.00 | 19.39 |
| ATOM | 4358 | NE1 | TRP | 215 | 22.681 | 6.037  | 4.606  | 1.00 | 19.10 |
| ATOM | 4359 | CE2 | TRP | 215 | 22.353 | 4.903  | 5.298  | 1.00 | 18.82 |
| ATOM | 4360 | CE3 | TRP | 215 | 20.347 | 3.722  | 5.960  | 1.00 | 20.69 |
| ATOM | 4361 | CZ2 | TRP | 215 | 23.173 | 3.953  | 5.918  | 1.00 | 19.47 |
| ATOM | 4362 | CZ3 | TRP | 215 | 21.165 | 2.777  | 6.578  | 1.00 | 19.60 |
| ATOM | 4363 | CH2 | TRP | 215 | 22.561 | 2.901  | 6.550  | 1.00 | 18.90 |
| ATOM | 4364 | H   | TRP | 215 | 19.602 | 9.070  | 5.419  | 1.00 | 0.00  |
| ATOM | 4365 | HE1 | TRP | 215 | 23.591 | 6.361  | 4.415  | 1.00 | 0.00  |
| ATOM | 4366 | N   | GLY | 216 | 17.937 | 5.800  | 6.890  | 1.00 | 24.62 |
| ATOM | 4367 | CA  | GLY | 216 | 17.860 | 5.346  | 8.267  | 1.00 | 28.30 |
| ATOM | 4368 | C   | GLY | 216 | 16.909 | 4.166  | 8.314  | 1.00 | 31.10 |
| ATOM | 4369 | O   | GLY | 216 | 16.172 | 3.942  | 7.356  | 1.00 | 32.33 |
| ATOM | 4370 | H   | GLY | 216 | 17.638 | 5.174  | 6.197  | 1.00 | 0.00  |
| ATOM | 4371 | N   | GLU | 217 | 16.910 | 3.415  | 9.408  | 1.00 | 32.47 |
| ATOM | 4372 | CA  | GLU | 217 | 16.031 | 2.257  | 9.530  | 1.00 | 33.88 |
| ATOM | 4373 | C   | GLU | 217 | 14.708 | 2.649  | 10.185 | 1.00 | 33.79 |
| ATOM | 4374 | O   | GLU | 217 | 14.481 | 2.364  | 11.360 | 1.00 | 35.74 |
| ATOM | 4375 | CB  | GLU | 217 | 16.721 | 1.163  | 10.350 | 1.00 | 36.85 |
| ATOM | 4376 | CG  | GLU | 217 | 18.154 | 0.887  | 9.923  | 1.00 | 41.77 |
| ATOM | 4377 | CD  | GLU | 217 | 18.363 | -0.527 | 9.416  | 1.00 | 45.44 |
| ATOM | 4378 | OE1 | GLU | 217 | 19.431 | -1.107 | 9.718  | 1.00 | 47.03 |
| ATOM | 4379 | OE2 | GLU | 217 | 17.477 | -1.050 | 8.701  | 1.00 | 47.68 |
| ATOM | 4380 | H   | GLU | 217 | 17.484 | 3.657  | 10.163 | 1.00 | 0.00  |
| ATOM | 4381 | N   | GLY | 219 | 13.827 | 3.294  | 9.428  | 1.00 | 32.19 |
| ATOM | 4382 | CA  | GLY | 219 | 12.550 | 3.707  | 9.985  | 1.00 | 30.79 |
| ATOM | 4383 | C   | GLY | 219 | 12.676 | 5.040  | 10.700 | 1.00 | 30.03 |
| ATOM | 4384 | O   | GLY | 219 | 13.785 | 5.469  | 11.022 | 1.00 | 29.00 |
| ATOM | 4385 | H   | GLY | 219 | 14.049 | 3.494  | 8.494  | 1.00 | 0.00  |
| ATOM | 4386 | N   | CYS | 220 | 11.541 | 5.686  | 10.958 | 1.00 | 29.77 |
| ATOM | 4387 | CA  | CYS | 220 | 11.520 | 6.986  | 11.627 | 1.00 | 28.30 |
| ATOM | 4388 | C   | CYS | 220 | 11.475 | 6.872  | 13.146 | 1.00 | 29.94 |
| ATOM | 4389 | O   | CYS | 220 | 10.662 | 6.112  | 13.694 | 1.00 | 30.48 |
| ATOM | 4390 | CB  | CYS | 220 | 10.333 | 7.808  | 11.144 | 1.00 | 23.84 |

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|------|------|------|-----|------|--------|--------|--------|------|-------|
| ATOM | 4391 | SG   | CYS | 220  | 10.284 | 7.985  | 9.346  | 1.00 | 19.78 |
| ATOM | 4392 | H    | CYS | 220  | 10.702 | 5.250  | 10.710 | 1.00 | 0.00  |
| ATOM | 4393 | N    | ALA | 221  | 12.354 | 7.628  | 13.811 | 1.00 | 29.90 |
| ATOM | 4394 | CA   | ALA | 221  | 12.458 | 7.650  | 15.267 | 1.00 | 29.71 |
| ATOM | 4395 | C    | ALA | 221  | 12.549 | 6.227  | 15.810 | 1.00 | 31.10 |
| ATOM | 4396 | O    | ALA | 221  | 11.733 | 5.809  | 16.637 | 1.00 | 32.62 |
| ATOM | 4397 | CB   | ALA | 221  | 11.269 | 8.387  | 15.865 | 1.00 | 27.85 |
| ATOM | 4398 | H    | ALA | 221  | 12.988 | 8.165  | 13.284 | 1.00 | 0.00  |
| ATOM | 4399 | N    | GLN | 221A | 13.537 | 5.481  | 15.322 | 1.00 | 32.09 |
| ATOM | 4400 | CA   | GLN | 221A | 13.726 | 4.092  | 15.729 | 1.00 | 33.10 |
| ATOM | 4401 | C    | GLN | 221A | 14.888 | 3.817  | 16.685 | 1.00 | 31.87 |
| ATOM | 4402 | O    | GLN | 221A | 15.994 | 4.348  | 16.529 | 1.00 | 31.97 |
| ATOM | 4403 | CB   | GLN | 221A | 13.822 | 3.177  | 14.502 | 1.00 | 35.62 |
| ATOM | 4404 | CG   | GLN | 221A | 12.486 | 2.943  | 13.800 | 1.00 | 39.24 |
| ATOM | 4405 | CD   | GLN | 221A | 11.448 | 2.312  | 14.714 | 1.00 | 41.06 |
| ATOM | 4406 | OE1  | GLN | 221A | 11.542 | 1.133  | 15.059 | 1.00 | 42.09 |
| ATOM | 4407 | NE2  | GLN | 221A | 10.465 | 3.102  | 15.128 | 1.00 | 42.62 |
| ATOM | 4408 | H    | GLN | 221A | 14.168 | 5.880  | 14.682 | 1.00 | 0.00  |
| ATOM | 4409 | HE21 | GLN | 221A | 10.471 | 4.045  | 14.843 | 1.00 | 0.00  |
| ATOM | 4410 | HE22 | GLN | 221A | 9.774  | 2.726  | 15.705 | 1.00 | 0.00  |
| ATOM | 4411 | N    | PRO | 222  | 14.637 | 2.970  | 17.694 | 1.00 | 30.49 |
| ATOM | 4412 | CA   | PRO | 222  | 15.579 | 2.549  | 18.735 | 1.00 | 29.25 |
| ATOM | 4413 | C    | PRO | 222  | 16.917 | 2.030  | 18.200 | 1.00 | 27.27 |
| ATOM | 4414 | O    | PRO | 222  | 16.962 | 1.005  | 17.525 | 1.00 | 27.31 |
| ATOM | 4415 | CB   | PRO | 222  | 14.803 | 1.445  | 19.449 | 1.00 | 30.64 |
| ATOM | 4416 | CG   | PRO | 222  | 13.390 | 1.931  | 19.357 | 1.00 | 30.41 |
| ATOM | 4417 | CD   | PRO | 222  | 13.306 | 2.373  | 17.926 | 1.00 | 30.24 |
| ATOM | 4418 | N    | ASN | 223  | 17.997 | 2.730  | 18.549 | 1.00 | 25.52 |
| ATOM | 4419 | CA   | ASN | 223  | 19.360 | 2.375  | 18.132 | 1.00 | 23.83 |
| ATOM | 4420 | C    | ASN | 223  | 19.575 | 2.522  | 16.627 | 1.00 | 22.48 |
| ATOM | 4421 | O    | ASN | 223  | 20.450 | 1.865  | 16.054 | 1.00 | 21.25 |
| ATOM | 4422 | CB   | ASN | 223  | 19.720 | 0.938  | 18.543 | 1.00 | 23.80 |
| ATOM | 4423 | CG   | ASN | 223  | 19.586 | 0.697  | 20.031 | 1.00 | 23.39 |
| ATOM | 4424 | OD1  | ASN | 223  | 18.854 | -0.191 | 20.461 | 1.00 | 22.89 |
| ATOM | 4425 | ND2  | ASN | 223  | 20.298 | 1.479  | 20.826 | 1.00 | 24.48 |
| ATOM | 4426 | H    | ASN | 223  | 17.842 | 3.514  | 19.109 | 1.00 | 0.00  |
| ATOM | 4427 | HD21 | ASN | 223  | 20.885 | 2.147  | 20.439 | 1.00 | 0.00  |
| ATOM | 4428 | HD22 | ASN | 223  | 20.183 | 1.323  | 21.787 | 1.00 | 0.00  |
| ATOM | 4429 | N    | ARG | 224  | 18.778 | 3.379  | 15.993 | 1.00 | 20.52 |
| ATOM | 4430 | CA   | ARG | 224  | 18.876 | 3.604  | 14.556 | 1.00 | 18.58 |
| ATOM | 4431 | C    | ARG | 224  | 18.616 | 5.068  | 14.214 | 1.00 | 17.70 |
| ATOM | 4432 | O    | ARG | 224  | 17.619 | 5.409  | 13.558 | 1.00 | 16.97 |
| ATOM | 4433 | CB   | ARG | 224  | 17.871 | 2.725  | 13.813 | 1.00 | 18.37 |
| ATOM | 4434 | CG   | ARG | 224  | 18.050 | 1.248  | 14.027 | 1.00 | 17.65 |
| ATOM | 4435 | CD   | ARG | 224  | 19.355 | 0.757  | 13.460 | 1.00 | 18.09 |
| ATOM | 4436 | NE   | ARG | 224  | 19.376 | -0.701 | 13.454 | 1.00 | 19.29 |
| ATOM | 4437 | CZ   | ARG | 224  | 19.832 | -1.452 | 14.451 | 1.00 | 18.79 |
| ATOM | 4438 | NH1  | ARG | 224  | 20.326 | -0.886 | 15.549 | 1.00 | 17.88 |
| ATOM | 4439 | NH2  | ARG | 224  | 19.748 | -2.774 | 14.371 | 1.00 | 18.85 |
| ATOM | 4440 | H    | ARG | 224  | 18.051 | 3.864  | 16.440 | 1.00 | 0.00  |
| ATOM | 4441 | HE   | ARG | 224  | 19.042 | -1.142 | 12.632 | 1.00 | 0.00  |
| ATOM | 4442 | HH11 | ARG | 224  | 20.402 | 0.110  | 15.662 | 1.00 | 0.00  |
| ATOM | 4443 | HH12 | ARG | 224  | 20.706 | -1.467 | 16.281 | 1.00 | 0.00  |
| ATOM | 4444 | HH21 | ARG | 224  | 19.350 | -3.266 | 13.576 | 1.00 | 0.00  |
| ATOM | 4445 | HH22 | ARG | 224  | 20.101 | -3.338 | 15.110 | 1.00 | 0.00  |
| ATOM | 4446 | N    | PRO | 225  | 19.513 | 5.956  | 14.663 | 1.00 | 16.47 |
| ATOM | 4447 | CA   | PRO | 225  | 19.378 | 7.388  | 14.401 | 1.00 | 15.04 |
| ATOM | 4448 | C    | PRO | 225  | 19.333 | 7.699  | 12.906 | 1.00 | 13.83 |
| ATOM | 4449 | O    | PRO | 225  | 19.834 | 6.927  | 12.080 | 1.00 | 13.63 |
| ATOM | 4450 | CB   | PRO | 225  | 20.625 | 7.972  | 15.076 | 1.00 | 14.51 |
| ATOM | 4451 | CG   | PRO | 225  | 21.616 | 6.867  | 14.995 | 1.00 | 13.40 |
| ATOM | 4452 | CD   | PRO | 225  | 20.775 | 5.677  | 15.368 | 1.00 | 15.83 |
| ATOM | 4453 | N    | GLY | 226  | 18.709 | 8.819  | 12.567 | 1.00 | 12.23 |

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|      |      |      |     |     |        |        |        |      |       |
|------|------|------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 4454 | CA   | GLY | 226 | 18.614 | 9.210  | 11.178 | 1.00 | 12.07 |
| ATOM | 4455 | C    | GLY | 226 | 19.983 | 9.560  | 10.654 | 1.00 | 13.32 |
| ATOM | 4456 | O    | GLY | 226 | 20.770 | 10.217 | 11.333 | 1.00 | 14.09 |
| ATOM | 4457 | H    | GLY | 226 | 18.298 | 9.413  | 13.228 | 1.00 | 0.00  |
| ATOM | 4458 | N    | ILE | 227 | 20.277 | 9.110  | 9.447  | 1.00 | 15.16 |
| ATOM | 4459 | CA   | ILE | 227 | 21.556 | 9.377  | 8.812  | 1.00 | 16.28 |
| ATOM | 4460 | C    | ILE | 227 | 21.389 | 10.501 | 7.788  | 1.00 | 17.99 |
| ATOM | 4461 | O    | ILE | 227 | 20.360 | 10.587 | 7.098  | 1.00 | 20.57 |
| ATOM | 4462 | CB   | ILE | 227 | 22.074 | 8.117  | 8.133  | 1.00 | 15.84 |
| ATOM | 4463 | CG1  | ILE | 227 | 22.294 | 7.042  | 9.197  | 1.00 | 16.01 |
| ATOM | 4464 | CG2  | ILE | 227 | 23.333 | 8.417  | 7.345  | 1.00 | 17.93 |
| ATOM | 4465 | H    | ILE | 227 | 19.608 | 8.622  | 8.929  | 1.00 | 0.00  |
| ATOM | 4466 | CD   | ILE | 227 | 22.887 | 5.775  | 8.672  | 1.00 | 16.80 |
| ATOM | 4467 | N    | TYR | 228 | 22.369 | 11.394 | 7.727  | 1.00 | 16.13 |
| ATOM | 4468 | CA   | TYR | 228 | 22.324 | 12.523 | 6.801  | 1.00 | 15.83 |
| ATOM | 4469 | C    | TYR | 228 | 23.617 | 12.529 | 5.995  | 1.00 | 17.09 |
| ATOM | 4470 | O    | TYR | 228 | 24.601 | 11.914 | 6.408  | 1.00 | 19.62 |
| ATOM | 4471 | CB   | TYR | 228 | 22.195 | 13.852 | 7.566  | 1.00 | 13.00 |
| ATOM | 4472 | CG   | TYR | 228 | 21.014 | 13.938 | 8.504  | 1.00 | 10.84 |
| ATOM | 4473 | CD1  | TYR | 228 | 20.874 | 13.032 | 9.549  | 1.00 | 11.77 |
| ATOM | 4474 | CD2  | TYR | 228 | 20.019 | 14.904 | 8.332  | 1.00 | 10.47 |
| ATOM | 4475 | CE1  | TYR | 228 | 19.776 | 13.068 | 10.399 | 1.00 | 13.52 |
| ATOM | 4476 | CE2  | TYR | 228 | 18.902 | 14.954 | 9.187  | 1.00 | 10.67 |
| ATOM | 4477 | CZ   | TYR | 228 | 18.791 | 14.024 | 10.216 | 1.00 | 12.88 |
| ATOM | 4478 | OH   | TYR | 228 | 17.701 | 14.003 | 11.059 | 1.00 | 13.55 |
| ATOM | 4479 | H    | TYR | 228 | 23.129 | 11.298 | 8.316  | 1.00 | 0.00  |
| ATOM | 4480 | HH   | TYR | 228 | 17.659 | 13.151 | 11.517 | 1.00 | 0.00  |
| ATOM | 4481 | N    | THR | 229 | 23.603 | 13.181 | 4.836  | 1.00 | 15.76 |
| ATOM | 4482 | CA   | THR | 229 | 24.788 | 13.270 | 3.959  | 1.00 | 14.93 |
| ATOM | 4483 | C    | THR | 229 | 25.632 | 14.408 | 4.519  | 1.00 | 15.41 |
| ATOM | 4484 | O    | THR | 229 | 25.136 | 15.520 | 4.724  | 1.00 | 17.46 |
| ATOM | 4485 | CB   | THR | 229 | 24.450 | 13.526 | 2.534  | 1.00 | 14.04 |
| ATOM | 4486 | OG1  | THR | 229 | 23.587 | 12.490 | 2.061  | 1.00 | 16.27 |
| ATOM | 4487 | CG2  | THR | 229 | 25.714 | 13.509 | 1.707  | 1.00 | 12.69 |
| ATOM | 4488 | H    | THR | 229 | 22.782 | 13.559 | 4.507  | 1.00 | 0.00  |
| ATOM | 4489 | HG1  | THR | 229 | 23.376 | 12.632 | 1.126  | 1.00 | 0.00  |
| ATOM | 4490 | N    | ARG | 230 | 26.908 | 14.124 | 4.733  | 1.00 | 14.43 |
| ATOM | 4491 | CA   | ARG | 230 | 27.851 | 15.094 | 5.257  | 1.00 | 14.26 |
| ATOM | 4492 | C    | ARG | 230 | 28.215 | 16.119 | 4.185  | 1.00 | 14.69 |
| ATOM | 4493 | O    | ARG | 230 | 28.953 | 15.826 | 3.241  | 1.00 | 13.22 |
| ATOM | 4494 | CB   | ARG | 230 | 29.063 | 14.332 | 5.771  | 1.00 | 16.36 |
| ATOM | 4495 | CG   | ARG | 230 | 30.115 | 15.164 | 6.396  | 1.00 | 18.75 |
| ATOM | 4496 | CD   | ARG | 230 | 30.927 | 14.395 | 7.377  | 1.00 | 22.90 |
| ATOM | 4497 | NE   | ARG | 230 | 30.362 | 14.535 | 8.709  | 1.00 | 26.74 |
| ATOM | 4498 | CZ   | ARG | 230 | 30.512 | 13.649 | 9.682  | 1.00 | 29.23 |
| ATOM | 4499 | NH1  | ARG | 230 | 31.214 | 12.547 | 9.457  | 1.00 | 31.14 |
| ATOM | 4500 | NH2  | ARG | 230 | 29.974 | 13.869 | 10.875 | 1.00 | 30.54 |
| ATOM | 4501 | H    | ARG | 230 | 27.249 | 13.236 | 4.480  | 1.00 | 0.00  |
| ATOM | 4502 | HE   | ARG | 230 | 29.832 | 15.330 | 8.865  | 1.00 | 0.00  |
| ATOM | 4503 | HH11 | ARG | 230 | 31.605 | 12.365 | 8.548  | 1.00 | 0.00  |
| ATOM | 4504 | HH12 | ARG | 230 | 31.295 | 11.854 | 10.170 | 1.00 | 0.00  |
| ATOM | 4505 | HH21 | ARG | 230 | 29.433 | 14.689 | 11.076 | 1.00 | 0.00  |
| ATOM | 4506 | HH22 | ARG | 230 | 30.020 | 13.174 | 11.603 | 1.00 | 0.00  |
| ATOM | 4507 | N    | VAL | 231 | 27.693 | 17.330 | 4.356  | 1.00 | 16.32 |
| ATOM | 4508 | CA   | VAL | 231 | 27.890 | 18.422 | 3.408  | 1.00 | 18.70 |
| ATOM | 4509 | C    | VAL | 231 | 29.314 | 18.873 | 3.134  | 1.00 | 20.24 |
| ATOM | 4510 | O    | VAL | 231 | 29.734 | 18.880 | 1.976  | 1.00 | 21.32 |
| ATOM | 4511 | CB   | VAL | 231 | 27.033 | 19.655 | 3.779  | 1.00 | 19.84 |
| ATOM | 4512 | CG1  | VAL | 231 | 27.144 | 20.732 | 2.709  | 1.00 | 19.33 |
| ATOM | 4513 | CG2  | VAL | 231 | 25.585 | 19.244 | 3.929  | 1.00 | 21.64 |
| ATOM | 4514 | H    | VAL | 231 | 27.171 | 17.503 | 5.169  | 1.00 | 0.00  |
| ATOM | 4515 | N    | THR | 232 | 30.046 | 19.288 | 4.164  | 1.00 | 21.65 |
| ATOM | 4516 | CA   | THR | 232 | 31.422 | 19.744 | 3.956  | 1.00 | 23.80 |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATL  | 4517 | C   | THR | 232 | 32.240 | 18.727 | 3.171  | 1.00 | 25.14 |
| ATOM | 4518 | O   | THR | 232 | 33.159 | 19.095 | 2.425  | 1.00 | 27.75 |
| ATOM | 4519 | C3  | THR | 232 | 32.173 | 20.107 | 5.270  | 1.00 | 24.30 |
| ATOM | 4520 | OG1 | THR | 232 | 32.263 | 18.971 | 6.134  | 1.00 | 23.79 |
| ATOM | 4521 | CG2 | THR | 232 | 31.484 | 21.237 | 5.999  | 1.00 | 24.90 |
| ATOM | 4522 | H   | THR | 232 | 29.663 | 19.242 | 5.059  | 1.00 | 0.00  |
| ATOM | 4523 | HG1 | THR | 232 | 32.896 | 19.290 | 6.796  | 1.00 | 0.00  |
| ATOM | 4524 | N   | TYR | 233 | 31.859 | 17.462 | 3.283  | 1.00 | 24.09 |
| ATOM | 4525 | CA  | TYR | 233 | 32.544 | 16.393 | 2.577  | 1.00 | 23.16 |
| ATOM | 4526 | C   | TYR | 233 | 32.434 | 16.581 | 1.063  | 1.00 | 22.61 |
| ATOM | 4527 | O   | TYR | 233 | 33.395 | 16.365 | 0.328  | 1.00 | 22.48 |
| ATOM | 4528 | CB  | TYR | 233 | 31.939 | 15.059 | 2.976  | 1.00 | 23.60 |
| ATOM | 4529 | CG  | TYR | 233 | 32.714 | 13.869 | 2.492  | 1.00 | 23.86 |
| ATOM | 4530 | CD1 | TYR | 233 | 33.472 | 13.104 | 3.376  | 1.00 | 24.73 |
| ATOM | 4531 | CD2 | TYR | 233 | 32.659 | 13.477 | 1.163  | 1.00 | 24.25 |
| ATOM | 4532 | CE1 | TYR | 233 | 34.149 | 11.977 | 2.947  | 1.00 | 24.67 |
| ATOM | 4533 | CE2 | TYR | 233 | 33.331 | 12.354 | 0.722  | 1.00 | 25.89 |
| ATOM | 4534 | CZ  | TYR | 233 | 34.071 | 11.607 | 1.617  | 1.00 | 25.90 |
| ATOM | 4535 | OH  | TYR | 233 | 34.704 | 10.469 | 1.181  | 1.00 | 28.31 |
| ATOM | 4536 | H   | TYR | 233 | 31.090 | 17.239 | 3.843  | 1.00 | 0.00  |
| ATOM | 4537 | HH  | TYR | 233 | 34.339 | 10.244 | 0.324  | 1.00 | 0.00  |
| ATOM | 4538 | N   | TYR | 234 | 31.256 | 16.969 | 0.592  | 1.00 | 22.65 |
| ATOM | 4539 | CA  | TYR | 234 | 31.055 | 17.172 | -0.835 | 1.00 | 21.87 |
| ATOM | 4540 | C   | TYR | 234 | 31.141 | 18.637 | -1.238 | 1.00 | 24.66 |
| ATOM | 4541 | O   | TYR | 234 | 30.781 | 18.995 | -2.367 | 1.00 | 27.00 |
| ATOM | 4542 | CB  | TYR | 234 | 29.731 | 16.550 | -1.293 | 1.00 | 16.86 |
| ATOM | 4543 | CG  | TYR | 234 | 29.766 | 15.044 | -1.260 | 1.00 | 12.21 |
| ATOM | 4544 | CD1 | TYR | 234 | 29.155 | 14.327 | -0.229 | 1.00 | 9.50  |
| ATOM | 4545 | CD2 | TYR | 234 | 30.474 | 14.334 | -2.224 | 1.00 | 10.43 |
| ATOM | 4546 | CE1 | TYR | 234 | 29.256 | 12.944 | -0.159 | 1.00 | 8.00  |
| ATOM | 4547 | CE2 | TYR | 234 | 30.583 | 12.953 | -2.164 | 1.00 | 9.47  |
| ATOM | 4548 | CZ  | TYR | 234 | 29.975 | 12.264 | -1.130 | 1.00 | 9.09  |
| ATOM | 4549 | OH  | TYR | 234 | 30.119 | 10.900 | -1.069 | 1.00 | 8.89  |
| ATOM | 4550 | H   | TYR | 234 | 30.527 | 17.138 | 1.235  | 1.00 | 0.00  |
| ATOM | 4551 | HH  | TYR | 234 | 30.936 | 10.600 | -1.455 | 1.00 | 0.00  |
| ATOM | 4552 | N   | LEU | 235 | 31.692 | 19.469 | -0.351 | 1.00 | 24.25 |
| ATOM | 4553 | CA  | LEU | 235 | 31.836 | 20.901 | -0.610 | 1.00 | 23.41 |
| ATOM | 4554 | C   | LEU | 235 | 32.494 | 21.264 | -1.930 | 1.00 | 23.12 |
| ATOM | 4555 | O   | LEU | 235 | 31.975 | 22.083 | -2.682 | 1.00 | 22.72 |
| ATOM | 4556 | CB  | LEU | 235 | 32.582 | 21.574 | 0.527  | 1.00 | 22.99 |
| ATOM | 4557 | CG  | LEU | 235 | 31.627 | 22.164 | 1.554  | 1.00 | 23.30 |
| ATOM | 4558 | CD1 | LEU | 235 | 32.420 | 22.847 | 2.636  | 1.00 | 24.61 |
| ATOM | 4559 | CD2 | LEU | 235 | 30.701 | 23.152 | 0.871  | 1.00 | 22.99 |
| ATOM | 4560 | H   | LEU | 235 | 32.004 | 19.104 | 0.505  | 1.00 | 0.00  |
| ATOM | 4561 | N   | ASP | 236 | 33.641 | 20.664 | -2.207 | 1.00 | 24.16 |
| ATOM | 4562 | CA  | ASP | 236 | 34.352 | 20.932 | -3.444 | 1.00 | 26.20 |
| ATOM | 4563 | C   | ASP | 236 | 33.496 | 20.564 | -4.642 | 1.00 | 26.26 |
| ATOM | 4564 | O   | ASP | 236 | 33.428 | 21.315 | -5.616 | 1.00 | 27.92 |
| ATOM | 4565 | CB  | ASP | 236 | 35.682 | 20.171 | -3.479 | 1.00 | 29.63 |
| ATOM | 4566 | CG  | ASP | 236 | 36.648 | 20.617 | -2.383 | 1.00 | 32.31 |
| ATOM | 4567 | OD1 | ASP | 236 | 37.623 | 19.884 | -2.121 | 1.00 | 33.53 |
| ATOM | 4568 | OD2 | ASP | 236 | 36.446 | 21.692 | -1.770 | 1.00 | 31.95 |
| ATOM | 4569 | H   | ASP | 236 | 34.045 | 20.070 | -1.544 | 1.00 | 0.00  |
| ATOM | 4570 | N   | TRP | 237 | 32.818 | 19.425 | -4.571 | 1.00 | 25.04 |
| ATOM | 4571 | CA  | TRP | 237 | 31.960 | 19.009 | -5.680 | 1.00 | 24.18 |
| ATOM | 4572 | C   | TRP | 237 | 30.837 | 20.029 | -5.870 | 1.00 | 23.27 |
| ATOM | 4573 | O   | TRP | 237 | 30.589 | 20.493 | -6.981 | 1.00 | 21.58 |
| ATOM | 4574 | CB  | TRP | 237 | 31.378 | 17.617 | -5.432 | 1.00 | 23.73 |
| ATOM | 4575 | CG  | TRP | 237 | 30.469 | 17.145 | -6.528 | 1.00 | 22.17 |
| ATOM | 4576 | CD1 | TRP | 237 | 30.836 | 16.592 | -7.723 | 1.00 | 22.93 |
| ATOM | 4577 | CD2 | TRP | 237 | 29.041 | 17.191 | -6.529 | 1.00 | 21.54 |
| ATOM | 4578 | NE1 | TRP | 237 | 29.722 | 16.293 | -8.468 | 1.00 | 22.96 |
| ATOM | 4579 | CE2 | TRP | 237 | 28.606 | 16.649 | -7.756 | 1.00 | 22.37 |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 4580 | CE3 | TRP | 237 | 28.083 | 17.640 | -5.610  | 1.00 | 20.65 |
| ATOM | 4581 | CZ2 | TRP | 237 | 27.253 | 16.544 | -8.085  | 1.00 | 21.65 |
| ATOM | 4582 | CZ3 | TRP | 237 | 26.746 | 17.535 | -5.939  | 1.00 | 19.81 |
| ATOM | 4583 | CH2 | TRP | 237 | 26.343 | 16.991 | -7.167  | 1.00 | 20.64 |
| ATOM | 4584 | H   | TRP | 237 | 32.895 | 18.884 | -3.759  | 1.00 | 0.00  |
| ATOM | 4585 | HE1 | TRP | 237 | 29.730 | 16.016 | -9.414  | 1.00 | 0.00  |
| ATOM | 4586 | N   | ILE | 238 | 30.185 | 20.391 | -4.773  | 1.00 | 23.25 |
| ATOM | 4587 | CA  | ILE | 238 | 29.117 | 21.371 | -4.815  | 1.00 | 24.34 |
| ATOM | 4588 | C   | ILE | 238 | 29.648 | 22.585 | -5.556  | 1.00 | 26.65 |
| ATOM | 4589 | O   | ILE | 238 | 29.093 | 22.997 | -6.574  | 1.00 | 26.58 |
| ATOM | 4590 | CB  | ILE | 238 | 28.706 | 21.803 | -3.391  | 1.00 | 23.89 |
| ATOM | 4591 | CG1 | ILE | 238 | 28.005 | 20.646 | -2.673  | 1.00 | 24.52 |
| ATOM | 4592 | CG2 | ILE | 238 | 27.819 | 23.042 | -3.439  | 1.00 | 22.20 |
| ATOM | 4593 | H   | ILE | 238 | 30.416 | 19.971 | -3.925  | 1.00 | 0.00  |
| ATOM | 4594 | CD  | ILE | 238 | 27.656 | 20.940 | -1.222  | 1.00 | 24.29 |
| ATOM | 4595 | N   | HIS | 239 | 30.792 | 23.077 | -5.091  | 1.00 | 29.74 |
| ATOM | 4596 | CA  | HIS | 239 | 31.436 | 24.254 | -5.662  | 1.00 | 31.99 |
| ATOM | 4597 | C   | HIS | 239 | 31.988 | 24.131 | -7.063  | 1.00 | 33.26 |
| ATOM | 4598 | O   | HIS | 239 | 32.538 | 25.099 | -7.586  | 1.00 | 33.88 |
| ATOM | 4599 | CB  | HIS | 239 | 32.503 | 24.791 | -4.718  | 1.00 | 32.75 |
| ATOM | 4600 | CG  | HIS | 239 | 31.933 | 25.432 | -3.497  | 1.00 | 34.71 |
| ATOM | 4601 | ND1 | HIS | 239 | 30.819 | 26.244 | -3.540  | 1.00 | 36.23 |
| ATOM | 4602 | CD2 | HIS | 239 | 32.293 | 25.357 | -2.195  | 1.00 | 35.47 |
| ATOM | 4603 | CE1 | HIS | 239 | 30.515 | 26.642 | -2.318  | 1.00 | 36.77 |
| ATOM | 4604 | NE2 | HIS | 239 | 31.395 | 26.117 | -1.484  | 1.00 | 37.64 |
| ATOM | 4605 | H   | HIS | 239 | 31.228 | 22.638 | -4.336  | 1.00 | 0.00  |
| ATOM | 4606 | HD1 | HIS | 239 | 30.354 | 26.506 | -4.374  | 1.00 | 0.00  |
| ATOM | 4607 | HE2 | HIS | 239 | 31.422 | 26.248 | -0.511  | 1.00 | 0.00  |
| ATOM | 4608 | N   | HIS | 240 | 31.857 | 22.951 | -7.664  | 1.00 | 34.03 |
| ATOM | 4609 | CA  | HIS | 240 | 32.309 | 22.746 | -9.036  | 1.00 | 35.29 |
| ATOM | 4610 | C   | HIS | 240 | 31.218 | 23.275 | -9.972  | 1.00 | 35.13 |
| ATOM | 4611 | O   | HIS | 240 | 31.440 | 23.469 | -11.168 | 1.00 | 34.59 |
| ATOM | 4612 | CB  | HIS | 240 | 32.543 | 21.255 | -9.328  | 1.00 | 38.17 |
| ATOM | 4613 | CG  | HIS | 240 | 33.767 | 20.677 | -8.682  | 1.00 | 39.96 |
| ATOM | 4614 | ND1 | HIS | 240 | 33.955 | 19.318 | -8.536  | 1.00 | 40.42 |
| ATOM | 4615 | CD2 | HIS | 240 | 34.870 | 21.266 | -8.164  | 1.00 | 40.33 |
| ATOM | 4616 | CE1 | HIS | 240 | 35.119 | 19.094 | -7.955  | 1.00 | 40.87 |
| ATOM | 4617 | NE2 | HIS | 240 | 35.694 | 20.258 | -7.721  | 1.00 | 41.52 |
| ATOM | 4618 | H   | HIS | 240 | 31.454 | 22.209 | -7.176  | 1.00 | 0.00  |
| ATOM | 4619 | HD1 | HIS | 240 | 33.335 | 18.625 | -8.848  | 1.00 | 0.00  |
| ATOM | 4620 | HE2 | HIS | 240 | 36.580 | 20.355 | -7.300  | 1.00 | 0.00  |
| ATOM | 4621 | N   | TYR | 241 | 30.027 | 23.479 | -9.418  | 1.00 | 35.72 |
| ATOM | 4622 | CA  | TYR | 241 | 28.894 | 23.968 | -10.187 | 1.00 | 35.80 |
| ATOM | 4623 | C   | TYR | 241 | 28.285 | 25.201 | -9.528  | 1.00 | 38.33 |
| ATOM | 4624 | O   | TYR | 241 | 27.910 | 26.149 | -10.210 | 1.00 | 40.03 |
| ATOM | 4625 | CB  | TYR | 241 | 27.835 | 22.873 | -10.300 | 1.00 | 32.91 |
| ATOM | 4626 | CG  | TYR | 241 | 28.385 | 21.545 | -10.750 | 1.00 | 29.73 |
| ATOM | 4627 | CD1 | TYR | 241 | 28.706 | 20.556 | -9.827  | 1.00 | 28.95 |
| ATOM | 4628 | CD2 | TYR | 241 | 28.584 | 21.277 | -12.098 | 1.00 | 29.38 |
| ATOM | 4629 | CE1 | TYR | 241 | 29.211 | 19.333 | -10.236 | 1.00 | 29.05 |
| ATOM | 4630 | CE2 | TYR | 241 | 29.086 | 20.055 | -12.522 | 1.00 | 28.77 |
| ATOM | 4631 | CZ  | TYR | 241 | 29.398 | 19.089 | -11.586 | 1.00 | 30.04 |
| ATOM | 4632 | OH  | TYR | 241 | 29.895 | 17.874 | -12.006 | 1.00 | 33.89 |
| ATOM | 4633 | H   | TYR | 241 | 29.878 | 23.277 | -8.471  | 1.00 | 0.00  |
| ATOM | 4634 | HH  | TYR | 241 | 29.959 | 17.872 | -12.962 | 1.00 | 0.00  |
| ATOM | 4635 | N   | VAL | 242 | 28.154 | 25.172 | -8.206  | 1.00 | 40.62 |
| ATOM | 4636 | CA  | VAL | 242 | 27.588 | 26.294 | -7.475  | 1.00 | 42.41 |
| ATOM | 4637 | C   | VAL | 242 | 28.696 | 27.295 | -7.190  | 1.00 | 46.20 |
| ATOM | 4638 | O   | VAL | 242 | 29.603 | 27.025 | -6.400  | 1.00 | 46.31 |
| ATOM | 4639 | CB  | VAL | 242 | 26.967 | 25.845 | -6.142  | 1.00 | 41.94 |
| ATOM | 4640 | CG1 | VAL | 242 | 26.193 | 26.992 | -5.525  | 1.00 | 41.57 |
| ATOM | 4641 | CG2 | VAL | 242 | 26.068 | 24.651 | -6.359  | 1.00 | 42.14 |
| ATOM | 4642 | H   | VAL | 242 | 28.450 | 24.382 | -7.715  | 1.00 | 0.00  |

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|      |      |     |     |     |        |         |         |      |       |
|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 4643 | N   | PRO | 243 | 28.628 | 28.473  | -7.817  | 1.00 | 49.97 |
| ATOM | 4644 | CA  | PRO | 243 | 29.628 | 29.528  | -7.641  | 1.00 | 53.66 |
| ATOM | 4645 | C   | PRO | 243 | 29.573 | 30.216  | -6.292  | 1.00 | 56.18 |
| ATOM | 4646 | O   | PRO | 243 | 28.499 | 30.564  | -5.797  | 1.00 | 55.01 |
| ATOM | 4647 | CB  | PRO | 243 | 29.296 | 30.493  | -8.769  | 1.00 | 53.76 |
| ATOM | 4648 | CG  | PRO | 243 | 27.810 | 30.379  | -8.871  | 1.00 | 53.31 |
| ATOM | 4649 | CD  | PRO | 243 | 27.603 | 28.880  | -8.795  | 1.00 | 52.08 |
| ATOM | 4650 | N   | LYS | 244 | 30.756 | 30.433  | -5.725  | 1.00 | 61.20 |
| ATOM | 4651 | CA  | LYS | 244 | 30.921 | 31.092  | -4.426  | 1.00 | 66.20 |
| ATOM | 4652 | C   | LYS | 244 | 30.562 | 32.575  | -4.582  | 1.00 | 68.75 |
| ATOM | 4653 | O   | LYS | 244 | 31.279 | 33.321  | -5.259  | 1.00 | 70.00 |
| ATOM | 4654 | CB  | LYS | 244 | 32.380 | 30.974  | -3.960  | 1.00 | 67.69 |
| ATOM | 4655 | CG  | LYS | 244 | 33.058 | 29.617  | -4.204  | 1.00 | 70.10 |
| ATOM | 4656 | CD  | LYS | 244 | 34.397 | 29.772  | -4.964  | 1.00 | 71.72 |
| ATOM | 4657 | CE  | LYS | 244 | 35.415 | 30.651  | -4.223  | 1.00 | 72.46 |
| ATOM | 4658 | NZ  | LYS | 244 | 36.721 | 30.806  | -4.949  | 1.00 | 72.45 |
| ATOM | 4659 | H   | LYS | 244 | 31.548 | 30.127  | -6.221  | 1.00 | 0.00  |
| ATOM | 4660 | HZ1 | LYS | 244 | 36.637 | 31.243  | -5.888  | 1.00 | 0.00  |
| ATOM | 4661 | HZ2 | LYS | 244 | 37.243 | 29.903  | -5.025  | 1.00 | 0.00  |
| ATOM | 4662 | HZ3 | LYS | 244 | 37.357 | 31.394  | -4.363  | 1.00 | 0.00  |
| ATOM | 4663 | N   | LYS | 245 | 29.467 | 32.994  | -3.948  | 1.00 | 69.97 |
| ATOM | 4664 | CA  | LYS | 245 | 29.011 | 34.384  | -4.038  | 1.00 | 70.61 |
| ATOM | 4665 | C   | LYS | 245 | 29.942 | 35.366  | -3.322  | 1.00 | 70.74 |
| ATOM | 4666 | O   | LYS | 245 | 29.810 | 36.585  | -3.474  | 1.00 | 70.46 |
| ATOM | 4667 | CB  | LYS | 245 | 27.584 | 34.512  | -3.493  | 1.00 | 70.94 |
| ATOM | 4668 | CG  | LYS | 245 | 26.861 | 35.790  | -3.889  | 1.00 | 70.89 |
| ATOM | 4669 | CD  | LYS | 245 | 26.500 | 35.817  | -5.376  | 1.00 | 70.82 |
| ATOM | 4670 | CE  | LYS | 245 | 25.729 | 37.074  | -5.730  | 1.00 | 70.84 |
| ATOM | 4671 | NZ  | LYS | 245 | 26.554 | 38.297  | -5.536  | 1.00 | 71.53 |
| ATOM | 4672 | H   | LYS | 245 | 28.975 | 32.332  | -3.428  | 1.00 | 0.00  |
| ATOM | 4673 | HZ1 | LYS | 245 | 27.373 | 38.301  | -6.193  | 1.00 | 0.00  |
| ATOM | 4674 | HZ2 | LYS | 245 | 26.874 | 38.252  | -4.541  | 1.00 | 0.00  |
| ATOM | 4675 | HZ3 | LYS | 245 | 25.938 | 39.122  | -5.691  | 1.00 | 0.00  |
| TER  | 4676 |     | LYS | 245 |        |         |         |      |       |
| ATOM | 4677 | N   | ILE | 16  | 8.225  | -15.885 | -10.143 | 1.00 | 24.22 |
| ATOM | 4678 | CA  | ILE | 16  | 8.964  | -16.235 | -11.350 | 1.00 | 23.21 |
| ATOM | 4679 | C   | ILE | 16  | 8.225  | -15.724 | -12.582 | 1.00 | 22.76 |
| ATOM | 4680 | O   | ILE | 16  | 7.140  | -16.216 | -12.928 | 1.00 | 23.91 |
| ATOM | 4681 | CB  | ILE | 16  | 9.171  | -17.776 | -11.455 | 1.00 | 22.54 |
| ATOM | 4682 | CG1 | ILE | 16  | 10.109 | -18.264 | -10.349 | 1.00 | 21.93 |
| ATOM | 4683 | CG2 | ILE | 16  | 9.727  | -18.157 | -12.821 | 1.00 | 22.41 |
| ATOM | 4684 | H   | ILE | 16  | 8.276  | -16.450 | -9.347  | 1.00 | 0.00  |
| ATOM | 4685 | CD  | ILE | 16  | 11.533 | -17.762 | -10.478 | 1.00 | 22.32 |
| ATOM | 4686 | N   | VAL | 17  | 8.818  | -14.742 | -13.248 | 1.00 | 21.78 |
| ATOM | 4687 | CA  | VAL | 17  | 8.232  | -14.165 | -14.449 | 1.00 | 21.80 |
| ATOM | 4688 | C   | VAL | 17  | 8.618  | -15.026 | -15.652 | 1.00 | 24.19 |
| ATOM | 4689 | O   | VAL | 17  | 9.691  | -15.640 | -15.666 | 1.00 | 25.28 |
| ATOM | 4690 | CB  | VAL | 17  | 8.742  | -12.718 | -14.680 | 1.00 | 20.14 |
| ATOM | 4691 | CG1 | VAL | 17  | 8.123  | -12.125 | -15.931 | 1.00 | 18.23 |
| ATOM | 4692 | CG2 | VAL | 17  | 8.436  | -11.846 | -13.472 | 1.00 | 19.55 |
| ATOM | 4693 | H   | VAL | 17  | 9.705  | -14.423 | -12.992 | 1.00 | 0.00  |
| ATOM | 4694 | N   | GLY | 18  | 7.693  | -15.148 | -16.603 | 1.00 | 25.93 |
| ATOM | 4695 | CA  | GLY | 18  | 7.942  | -15.902 | -17.826 | 1.00 | 28.43 |
| ATOM | 4696 | C   | GLY | 18  | 8.080  | -17.416 | -17.798 | 1.00 | 29.98 |
| ATOM | 4697 | O   | GLY | 18  | 8.018  | -18.059 | -18.847 | 1.00 | 29.76 |
| ATOM | 4698 | H   | GLY | 18  | 6.837  | -14.694 | -16.483 | 1.00 | 0.00  |
| ATOM | 4699 | N   | GLY | 19  | 8.291  | -17.998 | -16.626 | 1.00 | 31.39 |
| ATOM | 4700 | CA  | GLY | 19  | 8.430  | -19.439 | -16.564 | 1.00 | 33.60 |
| ATOM | 4701 | C   | GLY | 19  | 7.126  | -20.212 | -16.645 | 1.00 | 35.04 |
| ATOM | 4702 | O   | GLY | 19  | 6.054  | -19.636 | -16.874 | 1.00 | 34.94 |
| ATOM | 4703 | H   | GLY | 19  | 8.438  | -17.449 | -15.833 | 1.00 | 0.00  |
| ATOM | 4704 | N   | GLN | 20  | 7.219  | -21.509 | -16.363 | 1.00 | 35.65 |
| ATOM | 4705 | CA  | GLN | 20  | 6.084  | -22.423 | -16.374 | 1.00 | 35.51 |

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|      |      |      |     |    |        |         |         |      |       |
|------|------|------|-----|----|--------|---------|---------|------|-------|
| ATOM | 4706 | C    | GLN | 20 | 6.004  | -23.154 | -15.031 | 1.00 | 34.43 |
| ATOM | 4707 | O    | GLN | 20 | 6.811  | -22.909 | -14.132 | 1.00 | 33.71 |
| ATOM | 4708 | CB   | GLN | 20 | 6.226  | -23.429 | -17.520 | 1.00 | 37.81 |
| ATOM | 4709 | CG   | GLN | 20 | 7.594  | -24.097 | -17.607 | 1.00 | 42.23 |
| ATOM | 4710 | CD   | GLN | 20 | 7.596  | -25.337 | -18.492 | 1.00 | 44.42 |
| ATOM | 4711 | OE1  | GLN | 20 | 6.542  | -25.878 | -18.829 | 1.00 | 45.77 |
| ATOM | 4712 | NE2  | GLN | 20 | 8.790  | -25.806 | -18.854 | 1.00 | 45.05 |
| ATOM | 4713 | H    | GLN | 20 | 8.098  | -21.840 | -16.081 | 1.00 | 0.00  |
| ATOM | 4714 | HE21 | GLN | 20 | 9.605  | -25.358 | -18.559 | 1.00 | 0.00  |
| ATOM | 4715 | HE22 | GLN | 20 | 8.754  | -26.602 | -19.425 | 1.00 | 0.00  |
| ATOM | 4716 | N    | GLU | 21 | 5.023  | -24.037 | -14.893 | 1.00 | 34.17 |
| ATOM | 4717 | CA   | GLU | 21 | 4.834  | -24.797 | -13.662 | 1.00 | 33.73 |
| ATOM | 4718 | C    | GLU | 21 | 5.768  | -25.990 | -13.650 | 1.00 | 32.99 |
| ATOM | 4719 | O    | GLU | 21 | 5.836  | -26.748 | -14.614 | 1.00 | 34.12 |
| ATOM | 4720 | CB   | GLU | 21 | 3.388  | -25.257 | -13.557 | 1.00 | 36.71 |
| ATOM | 4721 | CG   | GLU | 21 | 3.063  | -25.984 | -12.275 | 1.00 | 41.14 |
| ATOM | 4722 | CD   | GLU | 21 | 1.571  | -26.064 | -12.004 | 1.00 | 42.78 |
| ATOM | 4723 | OE1  | GLU | 21 | 0.816  | -25.204 | -12.524 | 1.00 | 42.83 |
| ATOM | 4724 | OE2  | GLU | 21 | 1.161  | -26.975 | -11.243 | 1.00 | 44.63 |
| ATOM | 4725 | H    | GLU | 21 | 4.417  | -24.227 | -15.635 | 1.00 | 0.00  |
| ATOM | 4726 | N    | ALA | 22 | 6.499  | -26.150 | -12.560 | 1.00 | 32.41 |
| ATOM | 4727 | CA   | ALA | 22 | 7.459  | -27.235 | -12.446 | 1.00 | 32.78 |
| ATOM | 4728 | C    | ALA | 22 | 6.839  | -28.588 | -12.163 | 1.00 | 33.04 |
| ATOM | 4729 | O    | ALA | 22 | 5.869  | -28.696 | -11.415 | 1.00 | 33.60 |
| ATOM | 4730 | CB   | ALA | 22 | 8.492  | -26.909 | -11.385 | 1.00 | 33.32 |
| ATOM | 4731 | H    | ALA | 22 | 6.345  | -25.562 | -11.804 | 1.00 | 0.00  |
| ATOM | 4732 | N    | PRO | 23 | 7.397  | -29.647 | -12.769 | 1.00 | 33.44 |
| ATOM | 4733 | CA   | PRO | 23 | 6.917  | -31.016 | -12.589 | 1.00 | 33.21 |
| ATOM | 4734 | C    | PRO | 23 | 7.064  | -31.410 | -11.130 | 1.00 | 34.09 |
| ATOM | 4735 | O    | PRO | 23 | 8.002  | -30.979 | -10.452 | 1.00 | 33.58 |
| ATOM | 4736 | CB   | PRO | 23 | 7.861  | -31.815 | -13.481 | 1.00 | 33.05 |
| ATOM | 4737 | CG   | PRO | 23 | 8.158  | -30.850 | -14.592 | 1.00 | 32.20 |
| ATOM | 4738 | CD   | PRO | 23 | 8.432  | -29.595 | -13.816 | 1.00 | 33.28 |
| ATOM | 4739 | N    | ARG | 24 | 6.177  | -32.285 | -10.670 | 1.00 | 35.57 |
| ATOM | 4740 | CA   | ARG | 24 | 6.180  | -32.728 | -9.283  | 1.00 | 37.20 |
| ATOM | 4741 | C    | ARG | 24 | 7.431  | -33.486 | -8.880  | 1.00 | 37.27 |
| ATOM | 4742 | O    | ARG | 24 | 7.452  | -34.117 | -7.829  | 1.00 | 38.38 |
| ATOM | 4743 | CB   | ARG | 24 | 4.948  | -33.595 | -8.994  | 1.00 | 40.15 |
| ATOM | 4744 | CG   | ARG | 24 | 3.607  | -32.921 | -9.268  | 1.00 | 45.28 |
| ATOM | 4745 | CD   | ARG | 24 | 2.432  | -33.729 | -8.696  | 1.00 | 49.71 |
| ATOM | 4746 | NE   | ARG | 24 | 1.130  | -33.108 | -8.969  | 1.00 | 52.89 |
| ATOM | 4747 | CZ   | ARG | 24 | 0.368  | -32.500 | -8.057  | 1.00 | 54.67 |
| ATOM | 4748 | NH1  | ARG | 24 | 0.764  | -32.421 | -6.790  | 1.00 | 55.21 |
| ATOM | 4749 | NH2  | ARG | 24 | -0.785 | -31.947 | -8.422  | 1.00 | 54.77 |
| ATOM | 4750 | H    | ARG | 24 | 5.511  | -32.648 | -11.287 | 1.00 | 0.00  |
| ATOM | 4751 | HE   | ARG | 24 | 0.827  | -33.176 | -9.902  | 1.00 | 0.00  |
| ATOM | 4752 | HH11 | ARG | 24 | 1.633  | -32.843 | -6.521  | 1.00 | 0.00  |
| ATOM | 4753 | HH12 | ARG | 24 | 0.225  | -31.979 | -6.055  | 1.00 | 0.00  |
| ATOM | 4754 | HH21 | ARG | 24 | -1.097 | -31.948 | -9.375  | 1.00 | 0.00  |
| ATOM | 4755 | HH22 | ARG | 24 | -1.411 | -31.473 | -7.796  | 1.00 | 0.00  |
| ATOM | 4756 | N    | SER | 25 | 8.481  | -33.414 | -9.683  | 1.00 | 37.57 |
| ATOM | 4757 | CA   | SER | 25 | 9.704  | -34.136 | -9.367  | 1.00 | 39.11 |
| ATOM | 4758 | C    | SER | 25 | 10.979 | -33.303 | -9.385  | 1.00 | 38.90 |
| ATOM | 4759 | O    | SER | 25 | 11.880 | -33.521 | -8.575  | 1.00 | 40.61 |
| ATOM | 4760 | CB   | SER | 25 | 9.841  | -35.335 | -10.306 | 1.00 | 40.68 |
| ATOM | 4761 | OG   | SER | 25 | 9.230  | -35.067 | -11.563 | 1.00 | 42.48 |
| ATOM | 4762 | H    | SER | 25 | 8.497  | -32.924 | -10.512 | 1.00 | 0.00  |
| ATOM | 4763 | HG   | SER | 25 | 9.321  | -35.861 | -12.099 | 1.00 | 0.00  |
| ATOM | 4764 | N    | LYS | 26 | 11.053 | -32.346 | -10.303 | 1.00 | 37.21 |
| ATOM | 4765 | CA   | LYS | 26 | 12.227 | -31.494 | -10.423 | 1.00 | 35.38 |
| ATOM | 4766 | C    | LYS | 26 | 12.398 | -30.634 | -9.183  | 1.00 | 34.27 |
| ATOM | 4767 | O    | LYS | 26 | 11.489 | -30.521 | -8.365  | 1.00 | 33.98 |
| ATOM | 4768 | CB   | LYS | 26 | 12.098 | -30.584 | -11.643 | 1.00 | 36.26 |

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|      |      |      |     |    |        |         |         |      |       |
|------|------|------|-----|----|--------|---------|---------|------|-------|
| ATOM | 4769 | CG   | LYS | 26 | 12.068 | -31.308 | -12.978 | 1.00 | 38.84 |
| ATOM | 4770 | CD   | LYS | 26 | 13.463 | -31.638 | -13.514 | 1.00 | 41.20 |
| ATOM | 4771 | CE   | LYS | 26 | 14.149 | -30.425 | -14.158 | 1.00 | 42.09 |
| ATOM | 4772 | NZ   | LYS | 26 | 13.359 | -29.795 | -15.274 | 1.00 | 42.78 |
| ATOM | 4773 | H    | LYS | 26 | 10.275 | -32.203 | -10.876 | 1.00 | 0.00  |
| ATOM | 4774 | HZ1  | LYS | 26 | 12.476 | -29.375 | -14.914 | 1.00 | 0.00  |
| ATOM | 4775 | HZ2  | LYS | 26 | 13.117 | -30.450 | -16.042 | 1.00 | 0.00  |
| ATOM | 4776 | HZ3  | LYS | 26 | 13.894 | -29.002 | -15.682 | 1.00 | 0.00  |
| ATOM | 4777 | N    | TRP | 27 | 13.577 | -30.035 | -9.057  | 1.00 | 33.22 |
| ATOM | 4778 | CA   | TRP | 27 | 13.916 | -29.134 | -7.952  | 1.00 | 30.99 |
| ATOM | 4779 | C    | TRP | 27 | 13.588 | -29.693 | -6.576  | 1.00 | 30.71 |
| ATOM | 4780 | O    | TRP | 27 | 12.874 | -29.061 | -5.801  | 1.00 | 30.06 |
| ATOM | 4781 | CB   | TRP | 27 | 13.213 | -27.780 | -8.140  | 1.00 | 27.90 |
| ATOM | 4782 | CG   | TRP | 27 | 12.976 | -27.446 | -9.571  | 1.00 | 24.07 |
| ATOM | 4783 | CD1  | TRP | 27 | 11.782 | -27.135 | -10.148 | 1.00 | 23.26 |
| ATOM | 4784 | CD2  | TRP | 27 | 13.943 | -27.467 | -10.628 | 1.00 | 22.90 |
| ATOM | 4785 | NE1  | TRP | 27 | 11.944 | -26.966 | -11.501 | 1.00 | 23.64 |
| ATOM | 4786 | CE2  | TRP | 27 | 13.260 | -27.165 | -11.822 | 1.00 | 22.99 |
| ATOM | 4787 | CE3  | TRP | 27 | 15.320 | -27.721 | -10.682 | 1.00 | 22.99 |
| ATOM | 4788 | CZ2  | TRP | 27 | 13.906 | -27.108 | -13.061 | 1.00 | 21.66 |
| ATOM | 4789 | CZ3  | TRP | 27 | 15.965 | -27.666 | -11.919 | 1.00 | 21.66 |
| ATOM | 4790 | CH2  | TRP | 27 | 15.254 | -27.361 | -13.088 | 1.00 | 20.70 |
| ATOM | 4791 | H    | TRP | 27 | 14.257 | -30.217 | -9.734  | 1.00 | 0.00  |
| ATOM | 4792 | HE1  | TRP | 27 | 11.251 | -26.722 | -12.150 | 1.00 | 0.00  |
| ATOM | 4793 | N    | PRO | 28 | 14.138 | -30.872 | -6.242  | 1.00 | 31.61 |
| ATOM | 4794 | CA   | PRO | 28 | 13.904 | -31.524 | -4.947  | 1.00 | 32.51 |
| ATOM | 4795 | C    | PRO | 28 | 14.600 | -30.841 | -3.760  | 1.00 | 32.76 |
| ATOM | 4796 | O    | PRO | 28 | 14.372 | -31.203 | -2.604  | 1.00 | 33.56 |
| ATOM | 4797 | CB   | PRO | 28 | 14.453 | -32.931 | -5.181  | 1.00 | 32.50 |
| ATOM | 4798 | CG   | PRO | 28 | 15.589 | -32.685 | -6.106  | 1.00 | 32.27 |
| ATOM | 4799 | CD   | PRO | 28 | 14.994 | -31.712 | -7.099  | 1.00 | 32.31 |
| ATOM | 4800 | N    | TRP | 29 | 15.460 | -29.871 | -4.059  | 1.00 | 32.19 |
| ATOM | 4801 | CA   | TRP | 29 | 16.205 | -29.129 | -3.041  | 1.00 | 30.89 |
| ATOM | 4802 | C    | TRP | 29 | 15.497 | -27.841 | -2.631  | 1.00 | 30.76 |
| ATOM | 4803 | O    | TRP | 29 | 15.855 | -27.228 | -1.620  | 1.00 | 32.71 |
| ATOM | 4804 | CB   | TRP | 29 | 17.610 | -28.793 | -3.561  | 1.00 | 30.53 |
| ATOM | 4805 | CG   | TRP | 29 | 17.621 | -28.387 | -5.011  | 1.00 | 29.41 |
| ATOM | 4806 | CD1  | TRP | 29 | 17.257 | -27.176 | -5.532  | 1.00 | 28.36 |
| ATOM | 4807 | CD2  | TRP | 29 | 17.953 | -29.219 | -6.126  | 1.00 | 29.08 |
| ATOM | 4808 | NE1  | TRP | 29 | 17.333 | -27.207 | -6.902  | 1.00 | 28.19 |
| ATOM | 4809 | CE2  | TRP | 29 | 17.758 | -28.450 | -7.295  | 1.00 | 28.91 |
| ATOM | 4810 | CE3  | TRP | 29 | 18.392 | -30.543 | -6.251  | 1.00 | 29.08 |
| ATOM | 4811 | CZ2  | TRP | 29 | 17.988 | -28.958 | -8.575  | 1.00 | 29.45 |
| ATOM | 4812 | CZ3  | TRP | 29 | 18.622 | -31.050 | -7.524  | 1.00 | 30.79 |
| ATOM | 4813 | CH2  | TRP | 29 | 18.418 | -30.255 | -8.671  | 1.00 | 30.67 |
| ATOM | 4814 | H    | TRP | 29 | 15.588 | -29.644 | -4.996  | 1.00 | 0.00  |
| ATOM | 4815 | HE1  | TRP | 29 | 17.098 | -26.447 | -7.494  | 1.00 | 0.00  |
| ATOM | 4816 | N    | GLN | 30 | 14.524 | -27.420 | -3.439  | 1.00 | 27.97 |
| ATOM | 4817 | CA   | GLN | 30 | 13.762 | -26.202 | -3.188  | 1.00 | 25.07 |
| ATOM | 4818 | C    | GLN | 30 | 13.204 | -26.177 | -1.765  | 1.00 | 24.67 |
| ATOM | 4819 | O    | GLN | 30 | 12.725 | -27.190 | -1.257  | 1.00 | 25.19 |
| ATOM | 4820 | CB   | GLN | 30 | 12.637 | -26.073 | -4.222  | 1.00 | 23.69 |
| ATOM | 4821 | CG   | GLN | 30 | 11.840 | -24.770 | -4.164  | 1.00 | 22.42 |
| ATOM | 4822 | CD   | GLN | 30 | 12.716 | -23.531 | -4.261  | 1.00 | 21.52 |
| ATOM | 4823 | OE1  | GLN | 30 | 13.029 | -22.909 | -3.253  | 1.00 | 21.27 |
| ATOM | 4824 | NE2  | GLN | 30 | 13.121 | -23.176 | -5.471  | 1.00 | 19.76 |
| ATOM | 4825 | H    | GLN | 30 | 14.275 | -27.960 | -4.211  | 1.00 | 0.00  |
| ATOM | 4826 | HE21 | GLN | 30 | 12.895 | -23.724 | -6.248  | 1.00 | 0.00  |
| ATOM | 4827 | HE22 | GLN | 30 | 13.628 | -22.335 | -5.510  | 1.00 | 0.00  |
| ATOM | 4828 | N    | VAL | 31 | 13.307 | -25.021 | -1.119  | 1.00 | 23.83 |
| ATOM | 4829 | CA   | VAL | 31 | 12.825 | -24.827 | 0.242   | 1.00 | 22.84 |
| ATOM | 4830 | C    | VAL | 31 | 12.104 | -23.471 | 0.308   | 1.00 | 23.43 |
| ATOM | 4831 | O    | VAL | 31 | 12.461 | -22.534 | -0.411  | 1.00 | 23.85 |

|      |      |      |     |    |        |         |        |      |       |
|------|------|------|-----|----|--------|---------|--------|------|-------|
| ATOM | 4832 | CB   | VAL | 31 | 13.999 | -24.875 | 1.242  | 1.00 | 22.05 |
| ATOM | 4833 | CG1  | VAL | 31 | 13.555 | -24.432 | 2.614  | 1.00 | 21.32 |
| ATOM | 4834 | CG2  | VAL | 31 | 14.561 | -26.281 | 1.312  | 1.00 | 23.52 |
| ATOM | 4835 | H    | VAL | 31 | 13.690 | -24.239 | -1.572 | 1.00 | 0.00  |
| ATOM | 4836 | N    | SER | 32 | 11.068 | -23.388 | 1.140  | 1.00 | 21.70 |
| ATOM | 4837 | CA   | SER | 32 | 10.279 | -22.173 | 1.299  | 1.00 | 20.80 |
| ATOM | 4838 | C    | SER | 32 | 10.300 | -21.737 | 2.751  | 1.00 | 21.90 |
| ATOM | 4839 | O    | SER | 32 | 9.780  | -22.447 | 3.610  | 1.00 | 25.44 |
| ATOM | 4840 | CB   | SER | 32 | 8.831  | -22.446 | 0.870  | 1.00 | 21.01 |
| ATOM | 4841 | OG   | SER | 32 | 7.887  | -21.672 | 1.608  | 1.00 | 19.78 |
| ATOM | 4842 | H    | SER | 32 | 10.828 | -24.182 | 1.670  | 1.00 | 0.00  |
| ATOM | 4843 | HG   | SER | 32 | 8.016  | -21.955 | 2.527  | 1.00 | 0.00  |
| ATOM | 4844 | N    | LEU | 33 | 10.826 | -20.551 | 3.026  | 1.00 | 20.08 |
| ATOM | 4845 | CA   | LEU | 33 | 10.889 | -20.061 | 4.399  | 1.00 | 19.46 |
| ATOM | 4846 | C    | LEU | 33 | 9.567  | -19.421 | 4.828  | 1.00 | 19.50 |
| ATOM | 4847 | O    | LEU | 33 | 8.954  | -18.686 | 4.055  | 1.00 | 20.66 |
| ATOM | 4848 | CB   | LEU | 33 | 12.048 | -19.081 | 4.531  | 1.00 | 18.95 |
| ATOM | 4849 | CG   | LEU | 33 | 13.318 | -19.629 | 3.879  | 1.00 | 20.22 |
| ATOM | 4850 | CD1  | LEU | 33 | 14.491 | -18.709 | 4.167  | 1.00 | 21.54 |
| ATOM | 4851 | CD2  | LEU | 33 | 13.608 | -21.032 | 4.389  | 1.00 | 20.20 |
| ATOM | 4852 | H    | LEU | 33 | 11.146 | -19.972 | 2.315  | 1.00 | 0.00  |
| ATOM | 4853 | N    | ARG | 34 | 9.134  | -19.685 | 6.058  | 1.00 | 19.28 |
| ATOM | 4854 | CA   | ARG | 34 | 7.869  | -19.142 | 6.551  | 1.00 | 21.31 |
| ATOM | 4855 | C    | ARG | 34 | 8.039  | -18.293 | 7.795  | 1.00 | 23.91 |
| ATOM | 4856 | O    | ARG | 34 | 8.793  | -18.659 | 8.691  | 1.00 | 24.88 |
| ATOM | 4857 | CB   | ARG | 34 | 6.904  | -20.268 | 6.916  | 1.00 | 21.38 |
| ATOM | 4858 | CG   | ARG | 34 | 6.746  | -21.342 | 5.882  | 1.00 | 21.02 |
| ATOM | 4859 | CD   | ARG | 34 | 6.059  | -20.835 | 4.640  | 1.00 | 21.30 |
| ATOM | 4860 | NE   | ARG | 34 | 5.736  | -21.970 | 3.791  | 1.00 | 22.30 |
| ATOM | 4861 | CZ   | ARG | 34 | 4.626  | -22.698 | 3.897  | 1.00 | 21.20 |
| ATOM | 4862 | NH1  | ARG | 34 | 3.700  | -22.401 | 4.801  | 1.00 | 19.12 |
| ATOM | 4863 | NH2  | ARG | 34 | 4.467  | -23.764 | 3.131  | 1.00 | 21.55 |
| ATOM | 4864 | H    | ARG | 34 | 9.694  | -20.229 | 6.655  | 1.00 | 0.00  |
| ATOM | 4865 | HE   | ARG | 34 | 6.370  | -22.181 | 3.083  | 1.00 | 0.00  |
| ATOM | 4866 | HH11 | ARG | 34 | 3.743  | -21.598 | 5.401  | 1.00 | 0.00  |
| ATOM | 4867 | HH12 | ARG | 34 | 2.897  | -23.020 | 4.875  | 1.00 | 0.00  |
| ATOM | 4868 | HH21 | ARG | 34 | 5.049  | -24.171 | 2.420  | 1.00 | 0.00  |
| ATOM | 4869 | HH22 | ARG | 34 | 3.625  | -24.334 | 3.190  | 1.00 | 0.00  |
| ATOM | 4870 | N    | VAL | 35 | 7.310  | -17.181 | 7.859  | 1.00 | 25.82 |
| ATOM | 4871 | CA   | VAL | 35 | 7.336  | -16.288 | 9.020  | 1.00 | 27.27 |
| ATOM | 4872 | C    | VAL | 35 | 6.007  | -16.426 | 9.727  | 1.00 | 29.38 |
| ATOM | 4873 | O    | VAL | 35 | 4.959  | -16.507 | 9.083  | 1.00 | 29.92 |
| ATOM | 4874 | CB   | VAL | 35 | 7.486  | -14.794 | 8.650  | 1.00 | 27.28 |
| ATOM | 4875 | CG1  | VAL | 35 | 8.923  | -14.462 | 8.323  | 1.00 | 28.36 |
| ATOM | 4876 | CG2  | VAL | 35 | 6.557  | -14.427 | 7.507  | 1.00 | 27.09 |
| ATOM | 4877 | H    | VAL | 35 | 6.722  | -17.008 | 7.093  | 1.00 | 0.00  |
| ATOM | 4878 | N    | HIS | 36 | 6.033  | -16.445 | 11.049 | 1.00 | 31.91 |
| ATOM | 4879 | CA   | HIS | 36 | 4.798  | -16.575 | 11.777 | 1.00 | 35.58 |
| ATOM | 4880 | C    | HIS | 36 | 3.970  | -15.310 | 11.703 | 1.00 | 37.68 |
| ATOM | 4881 | O    | HIS | 36 | 4.236  | -14.341 | 12.413 | 1.00 | 39.26 |
| ATOM | 4882 | CB   | HIS | 36 | 5.027  | -16.946 | 13.234 | 1.00 | 38.28 |
| ATOM | 4883 | CG   | HIS | 36 | 3.760  | -17.262 | 13.962 | 1.00 | 42.80 |
| ATOM | 4884 | ND1  | HIS | 36 | 3.423  | -16.679 | 15.165 | 1.00 | 44.52 |
| ATOM | 4885 | CD2  | HIS | 36 | 2.718  | -18.062 | 13.625 | 1.00 | 44.67 |
| ATOM | 4886 | CE1  | HIS | 36 | 2.227  | -17.101 | 15.536 | 1.00 | 46.69 |
| ATOM | 4887 | NE2  | HIS | 36 | 1.777  | -17.941 | 14.619 | 1.00 | 46.59 |
| ATOM | 4888 | H    | HIS | 36 | 6.879  | -16.425 | 11.532 | 1.00 | 0.00  |
| ATOM | 4889 | HD1  | HIS | 36 | 3.981  | -16.042 | 15.661 | 1.00 | 0.00  |
| ATOM | 4890 | HE2  | HIS | 36 | 0.902  | -18.390 | 14.626 | 1.00 | 0.00  |
| ATOM | 4891 | N    | GLY | 37 | 2.994  | -15.315 | 10.804 | 1.00 | 38.63 |
| ATOM | 4892 | CA   | GLY | 37 | 2.099  | -14.185 | 10.664 | 1.00 | 37.93 |
| ATOM | 4893 | C    | GLY | 37 | 0.806  | -14.581 | 11.349 | 1.00 | 37.70 |
| ATOM | 4894 | O    | GLY | 37 | 0.831  | -15.321 | 12.340 | 1.00 | 37.76 |

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|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 4895 | H   | GLY | 37  | 2.868  | -16.076 | 10.207 | 1.00 | 0.00  |
| ATOM | 4896 | N   | PRO | 37A | -0.350 | -14.170 | 10.807 | 1.00 | 37.55 |
| ATOM | 4897 | CA  | PRO | 37A | -1.611 | -14.841 | 11.143 | 1.00 | 36.43 |
| ATOM | 4898 | C   | PRO | 37A | -1.496 | -16.338 | 10.841 | 1.00 | 35.22 |
| ATOM | 4899 | O   | PRO | 37A | -2.045 | -17.174 | 11.561 | 1.00 | 36.74 |
| ATOM | 4900 | CB  | PRO | 37A | -2.623 | -14.133 | 10.244 | 1.00 | 37.27 |
| ATOM | 4901 | CG  | PRO | 37A | -1.793 | -13.661 | 9.075  | 1.00 | 37.76 |
| ATOM | 4902 | CD  | PRO | 37A | -0.542 | -13.174 | 9.740  | 1.00 | 37.95 |
| ATOM | 4903 | N   | TYR | 37B | -0.751 | -16.654 | 9.785  | 1.00 | 31.47 |
| ATOM | 4904 | CA  | TYR | 37B | -0.494 | -18.025 | 9.380  | 1.00 | 27.72 |
| ATOM | 4905 | C   | TYR | 37B | 0.992  | -18.108 | 9.001  | 1.00 | 27.24 |
| ATOM | 4906 | O   | TYR | 37B | 1.722  | -17.129 | 9.146  | 1.00 | 27.56 |
| ATOM | 4907 | CB  | TYR | 37B | -1.406 | -18.425 | 8.222  | 1.00 | 24.95 |
| ATOM | 4908 | CG  | TYR | 37B | -1.240 | -17.610 | 6.964  | 1.00 | 22.80 |
| ATOM | 4909 | CD1 | TYR | 37B | -0.476 | -18.085 | 5.905  | 1.00 | 21.95 |
| ATOM | 4910 | CD2 | TYR | 37B | -1.852 | -16.372 | 6.825  | 1.00 | 21.38 |
| ATOM | 4911 | CE1 | TYR | 37B | -0.321 | -17.350 | 4.742  | 1.00 | 20.09 |
| ATOM | 4912 | CE2 | TYR | 37B | -1.704 | -15.628 | 5.662  | 1.00 | 20.24 |
| ATOM | 4913 | CZ  | TYR | 37B | -0.932 | -16.124 | 4.627  | 1.00 | 20.15 |
| ATOM | 4914 | OH  | TYR | 37B | -0.728 | -15.384 | 3.485  | 1.00 | 23.27 |
| ATOM | 4915 | H   | TYR | 37B | -0.328 | -15.952 | 9.256  | 1.00 | 0.00  |
| ATOM | 4916 | HH  | TYR | 37B | -1.119 | -14.500 | 3.605  | 1.00 | 0.00  |
| ATOM | 4917 | N   | TRP | 38  | 1.453  | -19.264 | 8.538  | 1.00 | 26.42 |
| ATOM | 4918 | CA  | TRP | 38  | 2.861  | -19.411 | 8.173  | 1.00 | 25.32 |
| ATOM | 4919 | C   | TRP | 38  | 3.143  | -19.032 | 6.728  | 1.00 | 23.23 |
| ATOM | 4920 | O   | TRP | 38  | 3.308  | -19.878 | 5.848  | 1.00 | 22.13 |
| ATOM | 4921 | CB  | TRP | 38  | 3.345  | -20.816 | 8.511  | 1.00 | 26.75 |
| ATOM | 4922 | CG  | TRP | 38  | 3.396  | -21.004 | 9.984  | 1.00 | 27.78 |
| ATOM | 4923 | CD1 | TRP | 38  | 2.393  | -21.462 | 10.790 | 1.00 | 28.33 |
| ATOM | 4924 | CD2 | TRP | 38  | 4.472  | -20.641 | 10.846 | 1.00 | 28.34 |
| ATOM | 4925 | NE1 | TRP | 38  | 2.778  | -21.395 | 12.104 | 1.00 | 28.40 |
| ATOM | 4926 | CE2 | TRP | 38  | 4.051  | -20.894 | 12.167 | 1.00 | 28.81 |
| ATOM | 4927 | CE3 | TRP | 38  | 5.756  | -20.121 | 10.631 | 1.00 | 28.65 |
| ATOM | 4928 | CZ2 | TRP | 38  | 4.869  | -20.643 | 13.273 | 1.00 | 29.76 |
| ATOM | 4929 | CZ3 | TRP | 38  | 6.567  | -19.873 | 11.729 | 1.00 | 28.85 |
| ATOM | 4930 | CH2 | TRP | 38  | 6.121  | -20.136 | 13.034 | 1.00 | 29.64 |
| ATOM | 4931 | H   | TRP | 38  | 0.849  | -20.023 | 8.414  | 1.00 | 0.00  |
| ATOM | 4932 | HE1 | TRP | 38  | 2.238  | -21.713 | 12.858 | 1.00 | 0.00  |
| ATOM | 4933 | N   | MET | 39  | 3.271  | -17.730 | 6.534  | 1.00 | 22.72 |
| ATOM | 4934 | CA  | MET | 39  | 3.490  | -17.119 | 5.239  | 1.00 | 23.27 |
| ATOM | 4935 | C   | MET | 39  | 4.864  | -17.339 | 4.635  | 1.00 | 23.29 |
| ATOM | 4936 | O   | MET | 39  | 5.882  | -17.268 | 5.328  | 1.00 | 24.37 |
| ATOM | 4937 | CB  | MET | 39  | 3.240  | -15.625 | 5.365  | 1.00 | 25.23 |
| ATOM | 4938 | CG  | MET | 39  | 2.782  | -14.948 | 4.100  | 1.00 | 29.13 |
| ATOM | 4939 | SD  | MET | 39  | 2.625  | -13.194 | 4.415  | 1.00 | 33.26 |
| ATOM | 4940 | CE  | MET | 39  | 1.762  | -13.226 | 6.043  | 1.00 | 32.18 |
| ATOM | 4941 | H   | MET | 39  | 3.279  | -17.157 | 7.333  | 1.00 | 0.00  |
| ATOM | 4942 | N   | HIS | 40  | 4.884  | -17.599 | 3.332  | 1.00 | 21.34 |
| ATOM | 4943 | CA  | HIS | 40  | 6.123  | -17.797 | 2.611  | 1.00 | 19.47 |
| ATOM | 4944 | C   | HIS | 40  | 6.668  | -16.419 | 2.300  | 1.00 | 19.04 |
| ATOM | 4945 | O   | HIS | 40  | 5.957  | -15.608 | 1.714  | 1.00 | 20.30 |
| ATOM | 4946 | CB  | HIS | 40  | 5.849  | -18.523 | 1.299  | 1.00 | 18.77 |
| ATOM | 4947 | CG  | HIS | 40  | 6.974  | -18.438 | 0.314  | 1.00 | 19.07 |
| ATOM | 4948 | ND1 | HIS | 40  | 7.985  | -19.370 | 0.257  | 1.00 | 19.43 |
| ATOM | 4949 | CD2 | HIS | 40  | 7.250  | -17.528 | -0.651 | 1.00 | 19.15 |
| ATOM | 4950 | CE1 | HIS | 40  | 8.836  | -19.041 | -0.698 | 1.00 | 19.74 |
| ATOM | 4951 | NE2 | HIS | 40  | 8.414  | -17.926 | -1.263 | 1.00 | 20.45 |
| ATOM | 4952 | H   | HIS | 40  | 4.066  | -17.639 | 2.808  | 1.00 | 0.00  |
| ATOM | 4953 | HD1 | HIS | 40  | 8.040  | -20.145 | 0.819  | 1.00 | 0.00  |
| ATOM | 4954 | HE2 | HIS | 40  | 8.911  | -17.400 | -1.939 | 1.00 | 0.00  |
| ATOM | 4955 | N   | PHE | 41  | 7.914  | -16.149 | 2.671  | 1.00 | 18.16 |
| ATOM | 4956 | CA  | PHE | 41  | 8.509  | -14.845 | 2.372  | 1.00 | 17.95 |
| ATOM | 4957 | C   | PHE | 41  | 9.726  | -14.898 | 1.428  | 1.00 | 17.52 |

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|      |      |     |     |    |        |         |        |      |       |
|------|------|-----|-----|----|--------|---------|--------|------|-------|
| ATOM | 4958 | O   | PHE | 41 | 9.977  | -13.966 | 0.667  | 1.00 | 16.15 |
| ATOM | 4959 | CB  | PHE | 41 | 8.816  | -14.068 | 3.660  | 1.00 | 18.97 |
| ATOM | 4960 | CG  | PHE | 41 | 9.829  | -14.726 | 4.569  | 1.00 | 20.64 |
| ATOM | 4961 | CD1 | PHE | 41 | 11.115 | -14.204 | 4.688  | 1.00 | 21.34 |
| ATOM | 4962 | CD2 | PHE | 41 | 9.487  | -15.823 | 5.345  | 1.00 | 21.60 |
| ATOM | 4963 | CE1 | PHE | 41 | 12.039 | -14.760 | 5.568  | 1.00 | 20.46 |
| ATOM | 4964 | CE2 | PHE | 41 | 10.409 | -16.383 | 6.229  | 1.00 | 22.18 |
| ATOM | 4965 | CZ  | PHE | 41 | 11.685 | -15.848 | 6.339  | 1.00 | 21.73 |
| ATOM | 4966 | H   | PHE | 41 | 8.388  | -16.849 | 3.171  | 1.00 | 0.00  |
| ATOM | 4967 | N   | CYS | 42 | 10.432 | -16.026 | 1.436  | 1.00 | 17.99 |
| ATOM | 4968 | CA  | CYS | 42 | 11.607 | -16.238 | 0.597  | 1.00 | 16.33 |
| ATOM | 4969 | C   | CYS | 42 | 11.792 | -17.723 | 0.372  | 1.00 | 16.40 |
| ATOM | 4970 | O   | CYS | 42 | 11.264 | -18.552 | 1.117  | 1.00 | 16.06 |
| ATOM | 4971 | CB  | CYS | 42 | 12.865 | -15.741 | 1.293  | 1.00 | 16.32 |
| ATOM | 4972 | SG  | CYS | 42 | 13.254 | -13.975 | 1.173  | 1.00 | 18.40 |
| ATOM | 4973 | H   | CYS | 42 | 10.180 | -16.756 | 2.032  | 1.00 | 0.00  |
| ATOM | 4974 | N   | GLY | 43 | 12.558 | -18.054 | -0.655 | 1.00 | 18.04 |
| ATOM | 4975 | CA  | GLY | 43 | 12.845 | -19.442 | -0.951 | 1.00 | 19.40 |
| ATOM | 4976 | C   | GLY | 43 | 14.209 | -19.797 | -0.374 | 1.00 | 20.79 |
| ATOM | 4977 | O   | GLY | 43 | 14.803 | -19.009 | 0.376  | 1.00 | 21.76 |
| ATOM | 4978 | H   | GLY | 43 | 13.017 | -17.350 | -1.154 | 1.00 | 0.00  |
| ATOM | 4979 | N   | GLY | 44 | 14.708 | -20.978 | -0.725 | 1.00 | 20.11 |
| ATOM | 4980 | CA  | GLY | 44 | 16.001 | -21.422 | -0.242 | 1.00 | 18.88 |
| ATOM | 4981 | C   | GLY | 44 | 16.275 | -22.778 | -0.845 | 1.00 | 19.33 |
| ATOM | 4982 | O   | GLY | 44 | 15.403 | -23.354 | -1.492 | 1.00 | 19.77 |
| ATOM | 4983 | H   | GLY | 44 | 14.188 | -21.585 | -1.300 | 1.00 | 0.00  |
| ATOM | 4984 | N   | SER | 45 | 17.482 | -23.290 | -0.653 | 1.00 | 19.85 |
| ATOM | 4985 | CA  | SER | 45 | 17.832 | -24.591 | -1.195 | 1.00 | 19.71 |
| ATOM | 4986 | C   | SER | 45 | 18.570 | -25.467 | -0.190 | 1.00 | 20.39 |
| ATOM | 4987 | O   | SER | 45 | 19.430 | -24.991 | 0.564  | 1.00 | 20.55 |
| ATOM | 4988 | CB  | SER | 45 | 18.656 | -24.425 | -2.473 | 1.00 | 20.24 |
| ATOM | 4989 | OG  | SER | 45 | 19.764 | -23.567 | -2.274 | 1.00 | 21.39 |
| ATOM | 4990 | H   | SER | 45 | 18.162 | -22.773 | -0.174 | 1.00 | 0.00  |
| ATOM | 4991 | HG  | SER | 45 | 19.497 | -22.652 | -2.116 | 1.00 | 0.00  |
| ATOM | 4992 | N   | LEU | 46 | 18.185 | -26.738 | -0.151 | 1.00 | 21.01 |
| ATOM | 4993 | CA  | LEU | 46 | 18.787 | -27.714 | 0.750  | 1.00 | 21.40 |
| ATOM | 4994 | C   | LEU | 46 | 20.149 | -28.092 | 0.185  | 1.00 | 22.72 |
| ATOM | 4995 | O   | LEU | 46 | 20.226 | -28.620 | -0.920 | 1.00 | 23.71 |
| ATOM | 4996 | CB  | LEU | 46 | 17.897 | -28.956 | 0.819  | 1.00 | 19.98 |
| ATOM | 4997 | CG  | LEU | 46 | 17.832 | -29.763 | 2.119  | 1.00 | 19.29 |
| ATOM | 4998 | CD1 | LEU | 46 | 17.160 | -28.939 | 3.210  | 1.00 | 17.03 |
| ATOM | 4999 | CD2 | LEU | 46 | 17.051 | -31.052 | 1.877  | 1.00 | 18.13 |
| ATOM | 5000 | H   | LEU | 46 | 17.445 | -27.020 | -0.719 | 1.00 | 0.00  |
| ATOM | 5001 | N   | ILE | 47 | 21.224 | -27.780 | 0.903  | 1.00 | 23.99 |
| ATOM | 5002 | CA  | ILE | 47 | 22.570 | -28.121 | 0.428  | 1.00 | 26.57 |
| ATOM | 5003 | C   | ILE | 47 | 23.197 | -29.207 | 1.298  | 1.00 | 28.97 |
| ATOM | 5004 | O   | ILE | 47 | 24.268 | -29.746 | 0.990  | 1.00 | 28.62 |
| ATOM | 5005 | CB  | ILE | 47 | 23.525 | -26.893 | 0.402  | 1.00 | 26.31 |
| ATOM | 5006 | CG1 | ILE | 47 | 23.666 | -26.277 | 1.801  | 1.00 | 25.50 |
| ATOM | 5007 | CG2 | ILE | 47 | 23.049 | -25.878 | -0.621 | 1.00 | 26.74 |
| ATOM | 5008 | H   | ILE | 47 | 21.125 | -27.356 | 1.786  | 1.00 | 0.00  |
| ATOM | 5009 | CD  | ILE | 47 | 24.813 | -25.290 | 1.931  | 1.00 | 22.85 |
| ATOM | 5010 | N   | HIS | 48 | 22.506 | -29.528 | 2.385  | 1.00 | 31.56 |
| ATOM | 5011 | CA  | HIS | 48 | 22.955 | -30.528 | 3.338  | 1.00 | 33.58 |
| ATOM | 5012 | C   | HIS | 48 | 21.701 | -30.909 | 4.121  | 1.00 | 33.17 |
| ATOM | 5013 | O   | HIS | 48 | 20.921 | -30.036 | 4.485  | 1.00 | 31.83 |
| ATOM | 5014 | CB  | HIS | 48 | 23.988 | -29.891 | 4.267  | 1.00 | 36.59 |
| ATOM | 5015 | CG  | HIS | 48 | 24.811 | -30.879 | 5.027  | 1.00 | 39.47 |
| ATOM | 5016 | ND1 | HIS | 48 | 25.914 | -31.499 | 4.481  | 1.00 | 41.12 |
| ATOM | 5017 | CD2 | HIS | 48 | 24.705 | -31.342 | 6.295  | 1.00 | 40.60 |
| ATOM | 5018 | CE1 | HIS | 48 | 26.453 | -32.303 | 5.379  | 1.00 | 42.20 |
| ATOM | 5019 | NE2 | HIS | 48 | 25.738 | -32.226 | 6.488  | 1.00 | 42.97 |
| ATOM | 5020 | H   | HIS | 48 | 21.670 | -29.050 | 2.589  | 1.00 | 0.00  |

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|      |      |      |     |    |        |         |        |      |       |
|------|------|------|-----|----|--------|---------|--------|------|-------|
| ATOM | 5021 | HD1  | HIS | 48 | 26.251 | -31.355 | 3.561  | 1.00 | 0.00  |
| ATOM | 5022 | HE2  | HIS | 48 | 25.904 | -32.699 | 7.334  | 1.00 | 0.00  |
| ATOM | 5023 | N    | PRO | 49 | 21.513 | -32.206 | 4.432  | 1.00 | 34.13 |
| ATOM | 5024 | CA   | PRO | 49 | 20.324 | -32.637 | 5.177  | 1.00 | 34.18 |
| ATOM | 5025 | C    | PRO | 49 | 20.021 | -31.832 | 6.439  | 1.00 | 34.75 |
| ATOM | 5026 | O    | PRO | 49 | 18.956 | -31.986 | 7.026  | 1.00 | 35.84 |
| ATOM | 5027 | CB   | PRO | 49 | 20.640 | -34.094 | 5.504  | 1.00 | 32.88 |
| ATOM | 5028 | CG   | PRO | 49 | 21.427 | -34.525 | 4.323  | 1.00 | 33.47 |
| ATOM | 5029 | CD   | PRO | 49 | 22.375 | -33.363 | 4.133  | 1.00 | 34.53 |
| ATOM | 5030 | N    | GLN | 50 | 20.934 | -30.961 | 6.849  | 1.00 | 33.89 |
| ATOM | 5031 | CA   | GLN | 50 | 20.703 | -30.175 | 8.044  | 1.00 | 34.31 |
| ATOM | 5032 | C    | GLN | 50 | 20.960 | -28.690 | 7.822  | 1.00 | 33.32 |
| ATOM | 5033 | O    | GLN | 50 | 20.608 | -27.862 | 8.659  | 1.00 | 33.87 |
| ATOM | 5034 | CB   | GLN | 50 | 21.583 | -30.707 | 9.170  | 1.00 | 35.88 |
| ATOM | 5035 | CG   | GLN | 50 | 21.173 | -30.262 | 10.558 | 1.00 | 37.87 |
| ATOM | 5036 | CD   | GLN | 50 | 21.970 | -30.967 | 11.631 | 1.00 | 39.08 |
| ATOM | 5037 | OE1  | GLN | 50 | 22.332 | -32.133 | 11.478 | 1.00 | 40.92 |
| ATOM | 5038 | NE2  | GLN | 50 | 22.255 | -30.268 | 12.718 | 1.00 | 40.07 |
| ATOM | 5039 | H    | GLN | 50 | 21.765 | -30.828 | 6.377  | 1.00 | 0.00  |
| ATOM | 5040 | HE21 | GLN | 50 | 21.911 | -29.345 | 12.764 | 1.00 | 0.00  |
| ATOM | 5041 | HE22 | GLN | 50 | 22.794 | -30.682 | 13.415 | 1.00 | 0.00  |
| ATOM | 5042 | N    | TRP | 51 | 21.516 | -28.349 | 6.668  | 1.00 | 31.53 |
| ATOM | 5043 | CA   | TRP | 51 | 21.824 | -26.960 | 6.358  | 1.00 | 30.74 |
| ATOM | 5044 | C    | TRP | 51 | 21.097 | -26.438 | 5.127  | 1.00 | 29.66 |
| ATOM | 5045 | O    | TRP | 51 | 21.157 | -27.048 | 4.053  | 1.00 | 30.66 |
| ATOM | 5046 | CB   | TRP | 51 | 23.329 | -26.793 | 6.168  | 1.00 | 31.96 |
| ATOM | 5047 | CG   | TRP | 51 | 24.098 | -26.805 | 7.441  | 1.00 | 32.01 |
| ATOM | 5048 | CD1  | TRP | 51 | 24.779 | -27.852 | 7.978  | 1.00 | 32.16 |
| ATOM | 5049 | CD2  | TRP | 51 | 24.289 | -25.699 | 8.330  | 1.00 | 31.96 |
| ATOM | 5050 | NE1  | TRP | 51 | 25.387 | -27.468 | 9.149  | 1.00 | 32.37 |
| ATOM | 5051 | CE2  | TRP | 51 | 25.103 | -26.152 | 9.387  | 1.00 | 31.28 |
| ATOM | 5052 | CE3  | TRP | 51 | 23.853 | -24.367 | 8.330  | 1.00 | 32.30 |
| ATOM | 5053 | CZ2  | TRP | 51 | 25.490 | -25.326 | 10.437 | 1.00 | 31.36 |
| ATOM | 5054 | CZ3  | TRP | 51 | 24.238 | -23.544 | 9.373  | 1.00 | 32.56 |
| ATOM | 5055 | CH2  | TRP | 51 | 25.051 | -24.030 | 10.414 | 1.00 | 32.51 |
| ATOM | 5056 | H    | TRP | 51 | 21.641 | -28.999 | 5.962  | 1.00 | 0.00  |
| ATOM | 5057 | HE1  | TRP | 51 | 25.936 | -28.019 | 9.748  | 1.00 | 0.00  |
| ATOM | 5058 | N    | VAL | 52 | 20.437 | -25.294 | 5.279  | 1.00 | 27.31 |
| ATOM | 5059 | CA   | VAL | 52 | 19.700 | -24.669 | 4.186  | 1.00 | 25.46 |
| ATOM | 5060 | C    | VAL | 52 | 20.420 | -23.399 | 3.747  | 1.00 | 24.59 |
| ATOM | 5061 | O    | VAL | 52 | 20.700 | -22.533 | 4.579  | 1.00 | 24.74 |
| ATOM | 5062 | CB   | VAL | 52 | 18.281 | -24.286 | 4.633  | 1.00 | 24.86 |
| ATOM | 5063 | CG1  | VAL | 52 | 17.455 | -23.866 | 3.443  | 1.00 | 25.37 |
| ATOM | 5064 | CG2  | VAL | 52 | 17.626 | -25.442 | 5.353  | 1.00 | 24.74 |
| ATOM | 5065 | H    | VAL | 52 | 20.428 | -24.868 | 6.157  | 1.00 | 0.00  |
| ATOM | 5066 | N    | LEU | 53 | 20.729 | -23.290 | 2.455  | 1.00 | 22.32 |
| ATOM | 5067 | CA   | LEU | 53 | 21.413 | -22.104 | 1.934  | 1.00 | 20.18 |
| ATOM | 5068 | C    | LEU | 53 | 20.380 | -21.128 | 1.401  | 1.00 | 20.59 |
| ATOM | 5069 | O    | LEU | 53 | 19.510 | -21.512 | 0.617  | 1.00 | 21.77 |
| ATOM | 5070 | CB   | LEU | 53 | 22.377 | -22.473 | 0.809  | 1.00 | 18.16 |
| ATOM | 5071 | CG   | LEU | 53 | 23.123 | -21.283 | 0.191  | 1.00 | 16.72 |
| ATOM | 5072 | CD1  | LEU | 53 | 24.193 | -20.778 | 1.146  | 1.00 | 14.83 |
| ATOM | 5073 | CD2  | LEU | 53 | 23.739 | -21.675 | -1.142 | 1.00 | 15.10 |
| ATOM | 5074 | H    | LEU | 53 | 20.446 | -23.975 | 1.817  | 1.00 | 0.00  |
| ATOM | 5075 | N    | THR | 54 | 20.485 | -19.870 | 1.812  | 1.00 | 20.55 |
| ATOM | 5076 | CA   | THR | 54 | 19.550 | -18.837 | 1.372  | 1.00 | 20.01 |
| ATOM | 5077 | C    | THR | 54 | 20.231 | -17.477 | 1.358  | 1.00 | 19.39 |
| ATOM | 5078 | O    | THR | 54 | 21.412 | -17.362 | 1.691  | 1.00 | 20.39 |
| ATOM | 5079 | CB   | THR | 54 | 18.307 | -18.776 | 2.289  | 1.00 | 20.29 |
| ATOM | 5080 | OG1  | THR | 54 | 17.451 | -17.708 | 1.876  | 1.00 | 21.02 |
| ATOM | 5081 | CG2  | THR | 54 | 18.713 | -18.554 | 3.726  | 1.00 | 20.72 |
| ATOM | 5082 | H    | THR | 54 | 21.209 | -19.604 | 2.421  | 1.00 | 0.00  |
| ATOM | 5083 | HG1  | THR | 54 | 16.839 | -17.495 | 2.587  | 1.00 | 0.00  |

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|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 5084 | N   | ALA | 55  | 19.490 | -16.449 | 0.962  | 1.00 | 17.67 |
| ATOM | 5085 | CA  | ALA | 55  | 20.025 | -15.098 | 0.905  | 1.00 | 17.14 |
| ATOM | 5086 | C   | ALA | 55  | 19.979 | -14.423 | 2.271  | 1.00 | 17.54 |
| ATOM | 5087 | O   | ALA | 55  | 19.022 | -14.586 | 3.021  | 1.00 | 18.30 |
| ATOM | 5088 | CB  | ALA | 55  | 19.265 | -14.277 | -0.114 | 1.00 | 16.70 |
| ATOM | 5089 | H   | ALA | 55  | 18.553 | -16.631 | 0.734  | 1.00 | 0.00  |
| ATOM | 5090 | N   | ALA | 56  | 20.988 | -13.609 | 2.556  | 1.00 | 17.90 |
| ATOM | 5091 | CA  | ALA | 56  | 21.090 | -12.907 | 3.826  | 1.00 | 16.90 |
| ATOM | 5092 | C   | ALA | 56  | 19.990 | -11.878 | 4.032  | 1.00 | 16.35 |
| ATOM | 5093 | O   | ALA | 56  | 19.515 | -11.697 | 5.150  | 1.00 | 17.82 |
| ATOM | 5094 | CB  | ALA | 56  | 22.453 | -12.244 | 3.946  | 1.00 | 17.02 |
| ATOM | 5095 | H   | ALA | 56  | 21.649 | -13.417 | 1.856  | 1.00 | 0.00  |
| ATOM | 5096 | N   | HIS | 57  | 19.552 | -11.228 | 2.958  | 1.00 | 15.40 |
| ATOM | 5097 | CA  | HIS | 57  | 18.508 | -10.207 | 3.080  | 1.00 | 15.38 |
| ATOM | 5098 | C   | HIS | 57  | 17.139 | -10.718 | 3.516  | 1.00 | 16.28 |
| ATOM | 5099 | O   | HIS | 57  | 16.265 | -9.932  | 3.877  | 1.00 | 15.88 |
| ATOM | 5100 | CB  | HIS | 57  | 18.392 | -9.362  | 1.805  | 1.00 | 13.79 |
| ATOM | 5101 | CG  | HIS | 57  | 17.631 | -10.011 | 0.689  | 1.00 | 10.94 |
| ATOM | 5102 | ND1 | HIS | 57  | 18.236 | -10.794 | -0.268 | 1.00 | 11.07 |
| ATOM | 5103 | CD2 | HIS | 57  | 16.333 | -9.908  | 0.319  | 1.00 | 10.95 |
| ATOM | 5104 | CE1 | HIS | 57  | 17.350 | -11.139 | -1.183 | 1.00 | 11.32 |
| ATOM | 5105 | NE2 | HIS | 57  | 16.186 | -10.613 | -0.850 | 1.00 | 10.68 |
| ATOM | 5106 | H   | HIS | 57  | 19.975 | -11.445 | 2.104  | 1.00 | 0.00  |
| ATOM | 5107 | HD1 | HIS | 57  | 19.191 | -11.020 | -0.331 | 1.00 | 0.00  |
| ATOM | 5108 | HE2 | HIS | 57  | 15.396 | -10.722 | -1.431 | 1.00 | 0.00  |
| ATOM | 5109 | N   | CYS | 58  | 16.946 | -12.029 | 3.458  | 1.00 | 17.59 |
| ATOM | 5110 | CA  | CYS | 58  | 15.690 | -12.622 | 3.875  | 1.00 | 18.87 |
| ATOM | 5111 | C   | CYS | 58  | 15.665 | -12.779 | 5.396  | 1.00 | 21.54 |
| ATOM | 5112 | O   | CYS | 58  | 14.600 | -12.801 | 6.008  | 1.00 | 23.63 |
| ATOM | 5113 | CB  | CYS | 58  | 15.503 | -13.991 | 3.218  | 1.00 | 17.28 |
| ATOM | 5114 | SG  | CYS | 58  | 15.275 | -13.954 | 1.410  | 1.00 | 19.05 |
| ATOM | 5115 | H   | CYS | 58  | 17.642 | -12.648 | 3.148  | 1.00 | 0.00  |
| ATOM | 5116 | N   | VAL | 59  | 16.840 | -12.832 | 6.014  | 1.00 | 22.88 |
| ATOM | 5117 | CA  | VAL | 59  | 16.918 | -13.031 | 7.455  | 1.00 | 23.96 |
| ATOM | 5118 | C   | VAL | 59  | 17.836 | -12.053 | 8.176  | 1.00 | 25.02 |
| ATOM | 5119 | O   | VAL | 59  | 18.079 | -12.203 | 9.372  | 1.00 | 25.80 |
| ATOM | 5120 | CB  | VAL | 59  | 17.372 | -14.480 | 7.777  | 1.00 | 24.67 |
| ATOM | 5121 | CG1 | VAL | 59  | 16.343 | -15.484 | 7.249  | 1.00 | 25.58 |
| ATOM | 5122 | CG2 | VAL | 59  | 18.736 | -14.769 | 7.149  | 1.00 | 23.78 |
| ATOM | 5123 | H   | VAL | 59  | 17.679 | -12.705 | 5.530  | 1.00 | 0.00  |
| ATOM | 5124 | N   | GLY | 60  | 18.324 | -11.046 | 7.456  | 1.00 | 25.55 |
| ATOM | 5125 | CA  | GLY | 60  | 19.216 | -10.063 | 8.045  | 1.00 | 26.64 |
| ATOM | 5126 | C   | GLY | 60  | 18.886 | -8.661  | 7.564  | 1.00 | 28.79 |
| ATOM | 5127 | O   | GLY | 60  | 17.790 | -8.437  | 7.049  | 1.00 | 30.03 |
| ATOM | 5128 | H   | GLY | 60  | 18.089 | -10.937 | 6.513  | 1.00 | 0.00  |
| ATOM | 5129 | N   | PRO | 60A | 19.781 | -7.679  | 7.752  | 1.00 | 29.70 |
| ATOM | 5130 | CA  | PRO | 60A | 20.906 | -7.702  | 8.692  | 1.00 | 30.78 |
| ATOM | 5131 | C   | PRO | 60A | 20.448 | -7.803  | 10.146 | 1.00 | 31.94 |
| ATOM | 5132 | O   | PRO | 60A | 21.149 | -8.371  | 10.980 | 1.00 | 31.27 |
| ATOM | 5133 | CB  | PRO | 60A | 21.597 | -6.368  | 8.419  | 1.00 | 31.02 |
| ATOM | 5134 | CG  | PRO | 60A | 20.457 | -5.477  | 8.005  | 1.00 | 30.15 |
| ATOM | 5135 | CD  | PRO | 60A | 19.702 | -6.374  | 7.068  | 1.00 | 29.37 |
| ATOM | 5136 | N   | ASP | 60B | 19.266 | -7.259  | 10.429 | 1.00 | 33.82 |
| ATOM | 5137 | CA  | ASP | 60B | 18.677 | -7.269  | 11.767 | 1.00 | 35.60 |
| ATOM | 5138 | C   | ASP | 60B | 18.375 | -8.677  | 12.248 | 1.00 | 36.50 |
| ATOM | 5139 | O   | ASP | 60B | 17.718 | -9.451  | 11.548 | 1.00 | 37.01 |
| ATOM | 5140 | CB  | ASP | 60B | 17.390 | -6.444  | 11.788 | 1.00 | 38.15 |
| ATOM | 5141 | CG  | ASP | 60B | 17.647 | -4.941  | 11.698 | 1.00 | 42.49 |
| ATOM | 5142 | OD1 | ASP | 60B | 18.487 | -4.412  | 12.469 | 1.00 | 42.50 |
| ATOM | 5143 | OD2 | ASP | 60B | 16.989 | -4.287  | 10.860 | 1.00 | 43.59 |
| ATOM | 5144 | H   | ASP | 60B | 18.768 | -6.801  | 9.725  | 1.00 | 0.00  |
| ATOM | 5145 | N   | VAL | 60C | 18.779 | -8.962  | 13.482 | 1.00 | 36.35 |
| ATOM | 5146 | CA  | VAL | 60C | 18.606 | -10.268 | 14.110 | 1.00 | 36.24 |

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|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 5147 | C   | VAL | 60C | 17.163 | -10.771 | 14.204 | 1.00 | 36.10 |
| ATOM | 5148 | O   | VAL | 60C | 16.315 | -10.142 | 14.830 | 1.00 | 35.49 |
| ATOM | 5149 | CB  | VAL | 60C | 19.249 | -10.265 | 15.510 | 1.00 | 36.43 |
| ATOM | 5150 | CG1 | VAL | 60C | 18.927 | -11.541 | 16.251 | 1.00 | 38.97 |
| ATOM | 5151 | CG2 | VAL | 60C | 20.751 | -10.109 | 15.382 | 1.00 | 37.33 |
| ATOM | 5152 | H   | VAL | 60C | 19.161 | -8.224  | 14.005 | 1.00 | 0.00  |
| ATOM | 5153 | N   | LYS | 60D | 16.907 | -11.928 | 13.597 | 1.00 | 36.82 |
| ATOM | 5154 | CA  | LYS | 60D | 15.583 | -12.547 | 13.600 | 1.00 | 37.98 |
| ATOM | 5155 | C   | LYS | 60D | 15.492 | -13.630 | 14.674 | 1.00 | 39.53 |
| ATOM | 5156 | O   | LYS | 60D | 16.514 | -14.095 | 15.187 | 1.00 | 40.12 |
| ATOM | 5157 | CB  | LYS | 60D | 15.264 | -13.158 | 12.224 | 1.00 | 37.38 |
| ATOM | 5158 | CG  | LYS | 60D | 14.513 | -12.232 | 11.252 | 1.00 | 37.34 |
| ATOM | 5159 | CD  | LYS | 60D | 15.332 | -11.006 | 10.888 | 1.00 | 37.20 |
| ATOM | 5160 | CE  | LYS | 60D | 14.470 | -9.875  | 10.356 | 1.00 | 36.94 |
| ATOM | 5161 | NZ  | LYS | 60D | 15.192 | -8.575  | 10.495 | 1.00 | 38.18 |
| ATOM | 5162 | H   | LYS | 60D | 17.656 | -12.419 | 13.202 | 1.00 | 0.00  |
| ATOM | 5163 | HZ1 | LYS | 60D | 16.099 | -8.642  | 9.991  | 1.00 | 0.00  |
| ATOM | 5164 | HZ2 | LYS | 60D | 15.451 | -8.402  | 11.490 | 1.00 | 0.00  |
| ATOM | 5165 | HZ3 | LYS | 60D | 14.662 | -7.755  | 10.144 | 1.00 | 0.00  |
| ATOM | 5166 | N   | ASP | 60E | 14.262 | -14.034 | 14.995 | 1.00 | 40.16 |
| ATOM | 5167 | CA  | ASP | 60E | 13.996 | -15.066 | 15.998 | 1.00 | 39.82 |
| ATOM | 5168 | C   | ASP | 60E | 13.752 | -16.418 | 15.323 | 1.00 | 38.83 |
| ATOM | 5169 | O   | ASP | 60E | 12.885 | -16.547 | 14.455 | 1.00 | 39.83 |
| ATOM | 5170 | CB  | ASP | 60E | 12.777 | -14.663 | 16.840 | 1.00 | 42.52 |
| ATOM | 5171 | CG  | ASP | 60E | 12.435 | -15.677 | 17.934 | 1.00 | 44.36 |
| ATOM | 5172 | OD1 | ASP | 60E | 13.213 | -16.625 | 18.170 | 1.00 | 45.50 |
| ATOM | 5173 | OD2 | ASP | 60E | 11.365 | -15.522 | 18.560 | 1.00 | 45.23 |
| ATOM | 5174 | H   | ASP | 60E | 13.490 | -13.645 | 14.547 | 1.00 | 0.00  |
| ATOM | 5175 | N   | LEU | 61  | 14.484 | -17.433 | 15.767 | 1.00 | 37.11 |
| ATOM | 5176 | CA  | LEU | 61  | 14.385 | -18.788 | 15.220 | 1.00 | 35.29 |
| ATOM | 5177 | C   | LEU | 61  | 13.000 | -19.400 | 15.426 | 1.00 | 34.96 |
| ATOM | 5178 | O   | LEU | 61  | 12.592 | -20.325 | 14.710 | 1.00 | 35.26 |
| ATOM | 5179 | CB  | LEU | 61  | 15.445 | -19.682 | 15.868 | 1.00 | 33.68 |
| ATOM | 5180 | CG  | LEU | 61  | 16.919 | -19.502 | 15.480 | 1.00 | 33.75 |
| ATOM | 5181 | CD1 | LEU | 61  | 17.316 | -18.042 | 15.419 | 1.00 | 33.54 |
| ATOM | 5182 | CD2 | LEU | 61  | 17.793 | -20.242 | 16.476 | 1.00 | 33.77 |
| ATOM | 5183 | H   | LEU | 61  | 15.064 | -17.243 | 16.534 | 1.00 | 0.00  |
| ATOM | 5184 | N   | ALA | 62  | 12.296 | -18.897 | 16.430 | 1.00 | 34.71 |
| ATOM | 5185 | CA  | ALA | 62  | 10.963 | -19.379 | 16.754 | 1.00 | 34.52 |
| ATOM | 5186 | C   | ALA | 62  | 9.939  | -18.718 | 15.857 | 1.00 | 34.16 |
| ATOM | 5187 | O   | ALA | 62  | 8.902  | -19.306 | 15.551 | 1.00 | 34.57 |
| ATOM | 5188 | CB  | ALA | 62  | 10.644 | -19.094 | 18.210 | 1.00 | 34.49 |
| ATOM | 5189 | H   | ALA | 62  | 12.676 | -18.174 | 16.981 | 1.00 | 0.00  |
| ATOM | 5190 | N   | ALA | 63  | 10.231 | -17.490 | 15.446 | 1.00 | 33.78 |
| ATOM | 5191 | CA  | ALA | 63  | 9.330  | -16.733 | 14.585 | 1.00 | 33.07 |
| ATOM | 5192 | C   | ALA | 63  | 9.252  | -17.318 | 13.187 | 1.00 | 32.15 |
| ATOM | 5193 | O   | ALA | 63  | 8.221  | -17.199 | 12.529 | 1.00 | 32.57 |
| ATOM | 5194 | CB  | ALA | 63  | 9.760  | -15.271 | 14.512 | 1.00 | 32.59 |
| ATOM | 5195 | H   | ALA | 63  | 11.060 | -17.066 | 15.757 | 1.00 | 0.00  |
| ATOM | 5196 | N   | LEU | 64  | 10.341 | -17.929 | 12.732 | 1.00 | 30.91 |
| ATOM | 5197 | CA  | LEU | 64  | 10.367 | -18.505 | 11.398 | 1.00 | 29.63 |
| ATOM | 5198 | C   | LEU | 64  | 10.468 | -20.021 | 11.384 | 1.00 | 29.35 |
| ATOM | 5199 | O   | LEU | 64  | 10.890 | -20.643 | 12.363 | 1.00 | 29.99 |
| ATOM | 5200 | CB  | LEU | 64  | 11.485 | -17.872 | 10.569 | 1.00 | 30.00 |
| ATOM | 5201 | CG  | LEU | 64  | 12.940 | -18.239 | 10.835 | 1.00 | 29.99 |
| ATOM | 5202 | CD1 | LEU | 64  | 13.394 | -19.193 | 9.748  | 1.00 | 31.32 |
| ATOM | 5203 | CD2 | LEU | 64  | 13.808 | -16.991 | 10.814 | 1.00 | 29.95 |
| ATOM | 5204 | H   | LEU | 64  | 11.133 | -17.978 | 13.300 | 1.00 | 0.00  |
| ATOM | 5205 | N   | ARG | 65  | 10.090 | -20.604 | 10.253 | 1.00 | 29.27 |
| ATOM | 5206 | CA  | ARG | 65  | 10.099 | -22.049 | 10.061 | 1.00 | 28.65 |
| ATOM | 5207 | C   | ARG | 65  | 10.597 | -22.362 | 8.648  | 1.00 | 25.23 |
| ATOM | 5208 | O   | ARG | 65  | 10.798 | -21.457 | 7.837  | 1.00 | 25.36 |
| ATOM | 5209 | CB  | ARG | 65  | 8.671  | -22.584 | 10.229 | 1.00 | 32.11 |

|      |      |      |     |    |        |         |        |      |       |
|------|------|------|-----|----|--------|---------|--------|------|-------|
| ATOM | 5210 | CG   | ARG | 65 | 8.534  | -23.862 | 11.044 | 1.00 | 36.70 |
| ATOM | 5211 | CD   | ARG | 65 | 8.240  | -23.593 | 12.517 | 1.00 | 39.44 |
| ATOM | 5212 | NE   | ARG | 65 | 9.362  | -22.948 | 13.193 | 1.00 | 43.47 |
| ATOM | 5213 | CZ   | ARG | 65 | 9.402  | -22.698 | 14.501 | 1.00 | 44.88 |
| ATOM | 5214 | NH1  | ARG | 65 | 8.370  | -23.039 | 15.269 | 1.00 | 44.04 |
| ATOM | 5215 | NH2  | ARG | 65 | 10.462 | -22.088 | 15.033 | 1.00 | 45.04 |
| ATOM | 5216 | H    | ARG | 65 | 9.782  | -20.026 | 9.525  | 1.00 | 0.00  |
| ATOM | 5217 | HE   | ARG | 65 | 10.108 | -22.615 | 12.643 | 1.00 | 0.00  |
| ATOM | 5218 | HH11 | ARG | 65 | 7.558  | -23.460 | 14.853 | 1.00 | 0.00  |
| ATOM | 5219 | HH12 | ARG | 65 | 8.343  | -22.855 | 16.256 | 1.00 | 0.00  |
| ATOM | 5220 | HH21 | ARG | 65 | 11.215 | -21.729 | 14.447 | 1.00 | 0.00  |
| ATOM | 5221 | HH22 | ARG | 65 | 10.534 | -21.873 | 16.005 | 1.00 | 0.00  |
| ATOM | 5222 | N    | VAL | 66 | 10.766 | -23.643 | 8.350  | 1.00 | 21.70 |
| ATOM | 5223 | CA   | VAL | 66 | 11.229 | -24.089 | 7.041  | 1.00 | 20.46 |
| ATOM | 5224 | C    | VAL | 66 | 10.324 | -25.204 | 6.525  | 1.00 | 21.48 |
| ATOM | 5225 | O    | VAL | 66 | 10.066 | -26.179 | 7.226  | 1.00 | 22.72 |
| ATOM | 5226 | CB   | VAL | 66 | 12.688 | -24.634 | 7.113  | 1.00 | 18.81 |
| ATOM | 5227 | CG1  | VAL | 66 | 13.088 | -25.295 | 5.811  | 1.00 | 16.33 |
| ATOM | 5228 | CG2  | VAL | 66 | 13.650 | -23.521 | 7.434  | 1.00 | 19.18 |
| ATOM | 5229 | H    | VAL | 66 | 10.618 | -24.321 | 9.036  | 1.00 | 0.00  |
| ATOM | 5230 | N    | GLN | 67 | 9.794  | -25.029 | 5.324  | 1.00 | 21.29 |
| ATOM | 5231 | CA   | GLN | 67 | 8.954  | -26.043 | 4.717  | 1.00 | 21.93 |
| ATOM | 5232 | C    | GLN | 67 | 9.736  | -26.563 | 3.525  | 1.00 | 22.16 |
| ATOM | 5233 | O    | GLN | 67 | 10.225 | -25.778 | 2.713  | 1.00 | 22.63 |
| ATOM | 5234 | CB   | GLN | 67 | 7.616  | -25.451 | 4.266  | 1.00 | 22.66 |
| ATOM | 5235 | CG   | GLN | 67 | 6.868  | -26.279 | 3.219  | 1.00 | 23.88 |
| ATOM | 5236 | CD   | GLN | 67 | 6.357  | -27.623 | 3.729  | 1.00 | 25.03 |
| ATOM | 5237 | OE1  | GLN | 67 | 7.028  | -28.314 | 4.493  | 1.00 | 25.74 |
| ATOM | 5238 | NE2  | GLN | 67 | 5.166  | -27.996 | 3.299  | 1.00 | 26.88 |
| ATOM | 5239 | H    | GLN | 67 | 9.947  | -24.208 | 4.810  | 1.00 | 0.00  |
| ATOM | 5240 | HE21 | GLN | 67 | 4.667  | -27.347 | 2.736  | 1.00 | 0.00  |
| ATOM | 5241 | HE22 | GLN | 67 | 4.788  | -28.873 | 3.476  | 1.00 | 0.00  |
| ATOM | 5242 | N    | LEU | 68 | 9.890  | -27.878 | 3.446  | 1.00 | 22.55 |
| ATOM | 5243 | CA   | LEU | 68 | 10.623 | -28.501 | 2.354  | 1.00 | 22.49 |
| ATOM | 5244 | C    | LEU | 68 | 9.829  | -28.505 | 1.056  | 1.00 | 22.83 |
| ATOM | 5245 | O    | LEU | 68 | 8.612  | -28.297 | 1.053  | 1.00 | 23.71 |
| ATOM | 5246 | CB   | LEU | 68 | 11.048 | -29.923 | 2.728  | 1.00 | 23.19 |
| ATOM | 5247 | CG   | LEU | 68 | 12.070 | -30.026 | 3.866  | 1.00 | 23.24 |
| ATOM | 5248 | CD1  | LEU | 68 | 12.418 | -31.477 | 4.132  | 1.00 | 23.29 |
| ATOM | 5249 | CD2  | LEU | 68 | 13.324 | -29.243 | 3.514  | 1.00 | 23.25 |
| ATOM | 5250 | H    | LEU | 68 | 9.445  | -28.424 | 4.131  | 1.00 | 0.00  |
| ATOM | 5251 | N    | ARG | 69 | 10.541 | -28.753 | -0.037 | 1.00 | 22.94 |
| ATOM | 5252 | CA   | ARG | 69 | 9.987  | -28.781 | -1.381 | 1.00 | 23.73 |
| ATOM | 5253 | C    | ARG | 69 | 8.608  | -29.396 | -1.466 | 1.00 | 24.51 |
| ATOM | 5254 | O    | ARG | 69 | 8.375  | -30.478 | -0.939 | 1.00 | 25.35 |
| ATOM | 5255 | CB   | ARG | 69 | 10.939 | -29.543 | -2.306 | 1.00 | 25.42 |
| ATOM | 5256 | CG   | ARG | 69 | 10.762 | -29.269 | -3.804 | 1.00 | 27.05 |
| ATOM | 5257 | CD   | ARG | 69 | 9.847  | -30.264 | -4.485 | 1.00 | 24.84 |
| ATOM | 5258 | NE   | ARG | 69 | 9.927  | -30.182 | -5.942 | 1.00 | 25.28 |
| ATOM | 5259 | CZ   | ARG | 69 | 8.922  | -29.804 | -6.730 | 1.00 | 27.02 |
| ATOM | 5260 | NH1  | ARG | 69 | 7.759  | -29.447 | -6.198 | 1.00 | 27.15 |
| ATOM | 5261 | NH2  | ARG | 69 | 9.036  | -29.872 | -8.052 | 1.00 | 26.49 |
| ATOM | 5262 | H    | ARG | 69 | 11.506 | -28.900 | 0.045  | 1.00 | 0.00  |
| ATOM | 5263 | HE   | ARG | 69 | 10.786 | -30.412 | -6.367 | 1.00 | 0.00  |
| ATOM | 5264 | HH11 | ARG | 69 | 7.632  | -29.437 | -5.210 | 1.00 | 0.00  |
| ATOM | 5265 | HH12 | ARG | 69 | 7.014  | -29.183 | -6.819 | 1.00 | 0.00  |
| ATOM | 5266 | HH21 | ARG | 69 | 9.876  | -30.222 | -8.458 | 1.00 | 0.00  |
| ATOM | 5267 | HH22 | ARG | 69 | 8.270  | -29.647 | -8.661 | 1.00 | 0.00  |
| ATOM | 5268 | N    | GLU | 70 | 7.698  | -28.689 | -2.128 | 1.00 | 26.15 |
| ATOM | 5269 | CA   | GLU | 70 | 6.324  | -29.149 | -2.330 | 1.00 | 27.28 |
| ATOM | 5270 | C    | GLU | 70 | 5.751  | -28.420 | -3.549 | 1.00 | 27.46 |
| ATOM | 5271 | O    | GLU | 70 | 6.263  | -27.372 | -3.949 | 1.00 | 26.86 |
| ATOM | 5272 | CB   | GLU | 70 | 5.462  | -28.881 | -1.096 | 1.00 | 26.84 |

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|      |      |      |     |    |        |         |        |      |       |
|------|------|------|-----|----|--------|---------|--------|------|-------|
| ATOM | 5273 | CG   | GLU | 70 | 5.212  | -27.421 | -0.845 | 1.00 | 26.37 |
| ATOM | 5274 | CD   | GLU | 70 | 4.344  | -27.182 | 0.357  | 1.00 | 26.20 |
| ATOM | 5275 | OE1  | GLU | 70 | 3.338  | -27.896 | 0.533  | 1.00 | 26.22 |
| ATOM | 5276 | OE2  | GLU | 70 | 4.672  | -26.262 | 1.123  | 1.00 | 27.39 |
| ATOM | 5277 | H    | GLU | 70 | 7.908  | -27.791 | -2.463 | 1.00 | 0.00  |
| ATOM | 5278 | N    | GLN | 71 | 4.717  | -28.990 | -4.159 | 1.00 | 28.05 |
| ATOM | 5279 | CA   | GLN | 71 | 4.122  | -28.384 | -5.347 | 1.00 | 28.30 |
| ATOM | 5280 | C    | GLN | 71 | 3.251  | -27.165 | -5.088 | 1.00 | 28.87 |
| ATOM | 5281 | O    | GLN | 71 | 3.266  | -26.219 | -5.880 | 1.00 | 29.84 |
| ATOM | 5282 | CB   | GLN | 71 | 3.307  | -29.410 | -6.145 | 1.00 | 27.42 |
| ATOM | 5283 | CG   | GLN | 71 | 4.126  | -30.375 | -6.980 | 1.00 | 26.65 |
| ATOM | 5284 | CD   | GLN | 71 | 4.835  | -29.720 | -8.158 | 1.00 | 26.68 |
| ATOM | 5285 | OE1  | GLN | 71 | 6.071  | -29.740 | -8.242 | 1.00 | 24.89 |
| ATOM | 5286 | NE2  | GLN | 71 | 4.059  | -29.157 | -9.083 | 1.00 | 25.94 |
| ATOM | 5287 | H    | GLN | 71 | 4.355  | -29.814 | -3.772 | 1.00 | 0.00  |
| ATOM | 5288 | HE21 | GLN | 71 | 3.087  | -29.106 | -9.032 | 1.00 | 0.00  |
| ATOM | 5289 | HE22 | GLN | 71 | 4.551  | -28.805 | -9.865 | 1.00 | 0.00  |
| ATOM | 5290 | N    | HIS | 72 | 2.479  | -27.189 | -4.005 | 1.00 | 27.97 |
| ATOM | 5291 | CA   | HIS | 72 | 1.580  | -26.081 | -3.709 | 1.00 | 27.88 |
| ATOM | 5292 | C    | HIS | 72 | 1.780  | -25.461 | -2.332 | 1.00 | 28.94 |
| ATOM | 5293 | O    | HIS | 72 | 1.205  | -25.900 | -1.335 | 1.00 | 27.69 |
| ATOM | 5294 | CB   | HIS | 72 | 0.138  | -26.529 | -3.910 | 1.00 | 26.91 |
| ATOM | 5295 | CG   | HIS | 72 | -0.131 | -27.067 | -5.277 | 1.00 | 25.69 |
| ATOM | 5296 | ND1  | HIS | 72 | -0.480 | -26.261 | -6.336 | 1.00 | 25.93 |
| ATOM | 5297 | CD2  | HIS | 72 | -0.053 | -28.325 | -5.771 | 1.00 | 25.84 |
| ATOM | 5298 | CE1  | HIS | 72 | -0.601 | -26.994 | -7.427 | 1.00 | 26.06 |
| ATOM | 5299 | NE2  | HIS | 72 | -0.346 | -28.251 | -7.111 | 1.00 | 27.28 |
| ATOM | 5300 | H    | HIS | 72 | 2.542  | -27.897 | -3.328 | 1.00 | 0.00  |
| ATOM | 5301 | HD1  | HIS | 72 | -0.597 | -25.290 | -6.267 | 1.00 | 0.00  |
| ATOM | 5302 | HE2  | HIS | 72 | -0.369 | -28.973 | -7.776 | 1.00 | 0.00  |
| ATOM | 5303 | N    | LEU | 73 | 2.492  | -24.339 | -2.347 | 1.00 | 31.53 |
| ATOM | 5304 | CA   | LEU | 73 | 2.866  | -23.568 | -1.169 | 1.00 | 33.59 |
| ATOM | 5305 | C    | LEU | 73 | 2.317  | -23.839 | 0.225  | 1.00 | 36.07 |
| ATOM | 5306 | O    | LEU | 73 | 3.102  | -24.148 | 1.114  | 1.00 | 39.04 |
| ATOM | 5307 | CB   | LEU | 73 | 2.789  | -22.070 | -1.452 | 1.00 | 32.56 |
| ATOM | 5308 | CG   | LEU | 73 | 4.150  | -21.379 | -1.565 | 1.00 | 31.47 |
| ATOM | 5309 | CD1  | LEU | 73 | 3.940  | -19.892 | -1.810 | 1.00 | 32.49 |
| ATOM | 5310 | CD2  | LEU | 73 | 4.978  | -21.609 | -0.301 | 1.00 | 30.25 |
| ATOM | 5311 | H    | LEU | 73 | 2.769  | -23.988 | -3.218 | 1.00 | 0.00  |
| ATOM | 5312 | N    | TYR | 74 | 1.016  | -23.674 | 0.460  | 1.00 | 35.27 |
| ATOM | 5313 | CA   | TYR | 74 | 0.496  | -23.873 | 1.817  | 1.00 | 35.63 |
| ATOM | 5314 | C    | TYR | 74 | -0.400 | -25.083 | 2.050  | 1.00 | 38.84 |
| ATOM | 5315 | O    | TYR | 74 | -0.816 | -25.341 | 3.182  | 1.00 | 39.81 |
| ATOM | 5316 | CB   | TYR | 74 | -0.249 | -22.621 | 2.294  | 1.00 | 32.31 |
| ATOM | 5317 | CG   | TYR | 74 | 0.495  | -21.327 | 2.081  | 1.00 | 30.31 |
| ATOM | 5318 | CD1  | TYR | 74 | 0.379  | -20.633 | 0.881  | 1.00 | 30.17 |
| ATOM | 5319 | CD2  | TYR | 74 | 1.310  | -20.793 | 3.078  | 1.00 | 29.05 |
| ATOM | 5320 | CE1  | TYR | 74 | 1.058  | -19.441 | 0.677  | 1.00 | 29.66 |
| ATOM | 5321 | CE2  | TYR | 74 | 1.990  | -19.598 | 2.884  | 1.00 | 27.82 |
| ATOM | 5322 | CZ   | TYR | 74 | 1.860  | -18.928 | 1.681  | 1.00 | 28.80 |
| ATOM | 5323 | OH   | TYR | 74 | 2.520  | -17.735 | 1.474  | 1.00 | 30.33 |
| ATOM | 5324 | H    | TYR | 74 | 0.413  | -23.450 | -0.263 | 1.00 | 0.00  |
| ATOM | 5325 | HH   | TYR | 74 | 2.489  | -17.232 | 2.293  | 1.00 | 0.00  |
| ATOM | 5326 | N    | TYR | 75 | -0.709 | -25.838 | 1.006  | 1.00 | 42.14 |
| ATOM | 5327 | CA   | TYR | 75 | -1.590 | -26.977 | 1.187  | 1.00 | 44.60 |
| ATOM | 5328 | C    | TYR | 75 | -0.829 | -28.283 | 1.332  | 1.00 | 45.33 |
| ATOM | 5329 | O    | TYR | 75 | -0.297 | -28.837 | 0.364  | 1.00 | 45.82 |
| ATOM | 5330 | CB   | TYR | 75 | -2.693 | -26.948 | 0.115  | 1.00 | 47.59 |
| ATOM | 5331 | CG   | TYR | 75 | -3.027 | -28.203 | -0.653 | 1.00 | 50.92 |
| ATOM | 5332 | CD1  | TYR | 75 | -3.989 | -29.105 | -0.185 | 1.00 | 52.26 |
| ATOM | 5333 | CD2  | TYR | 75 | -2.491 | -28.413 | -1.925 | 1.00 | 53.02 |
| ATOM | 5334 | CE1  | TYR | 75 | -4.420 | -30.178 | -0.978 | 1.00 | 54.44 |
| ATOM | 5335 | CE2  | TYR | 75 | -2.911 | -29.476 | -2.727 | 1.00 | 54.89 |

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|------|------|------|-----|----|--------|---------|--------|------|-------|
| ATOM | 5336 | CZ   | TYR | 75 | -3.878 | -30.353 | -2.254 | 1.00 | 54.87 |
| ATOM | 5337 | OH   | TYR | 75 | -4.332 | -31.361 | -3.080 | 1.00 | 53.68 |
| ATOM | 5338 | H    | TYR | 75 | -0.236 | -25.700 | 0.161  | 1.00 | 0.00  |
| ATOM | 5339 | HH   | TYR | 75 | -4.152 | -31.155 | -4.002 | 1.00 | 0.00  |
| ATOM | 5340 | N    | GLN | 79 | -0.738 | -28.694 | 2.599  | 1.00 | 45.60 |
| ATOM | 5341 | CA   | GLN | 79 | -0.054 | -29.895 | 3.094  | 1.00 | 45.61 |
| ATOM | 5342 | C    | GLN | 79 | 1.367  | -29.598 | 3.580  | 1.00 | 43.77 |
| ATOM | 5343 | O    | GLN | 79 | 2.350  | -30.188 | 3.124  | 1.00 | 43.51 |
| ATOM | 5344 | CB   | GLN | 79 | -0.105 | -31.067 | 2.103  | 1.00 | 47.43 |
| ATOM | 5345 | CG   | GLN | 79 | -1.449 | -31.801 | 2.135  | 1.00 | 50.20 |
| ATOM | 5346 | CD   | GLN | 79 | -1.484 | -33.048 | 1.259  | 1.00 | 52.53 |
| ATOM | 5347 | OE1  | GLN | 79 | -2.469 | -33.793 | 1.266  | 1.00 | 53.26 |
| ATOM | 5348 | NE2  | GLN | 79 | -0.414 | -33.281 | 0.501  | 1.00 | 52.61 |
| ATOM | 5349 | H    | GLN | 79 | -1.122 | -28.087 | 3.270  | 1.00 | 0.00  |
| ATOM | 5350 | HE21 | GLN | 79 | 0.367  | -32.685 | 0.505  | 1.00 | 0.00  |
| ATOM | 5351 | HE22 | GLN | 79 | -0.467 | -34.082 | -0.053 | 1.00 | 0.00  |
| ATOM | 5352 | N    | ASP | 80 | 1.433  | -28.704 | 4.561  | 1.00 | 41.53 |
| ATOM | 5353 | CA   | ASP | 80 | 2.680  | -28.274 | 5.168  | 1.00 | 39.70 |
| ATOM | 5354 | C    | ASP | 80 | 3.221  | -29.229 | 6.207  | 1.00 | 39.35 |
| ATOM | 5355 | O    | ASP | 80 | 2.479  | -29.951 | 6.870  | 1.00 | 38.96 |
| ATOM | 5356 | CB   | ASP | 80 | 2.517  | -26.896 | 5.817  | 1.00 | 38.57 |
| ATOM | 5357 | CG   | ASP | 80 | 2.666  | -25.762 | 4.828  | 1.00 | 36.42 |
| ATOM | 5358 | OD1  | ASP | 80 | 3.299  | -25.979 | 3.780  | 1.00 | 34.50 |
| ATOM | 5359 | OD2  | ASP | 80 | 2.169  | -24.647 | 5.108  | 1.00 | 34.84 |
| ATOM | 5360 | H    | ASP | 80 | 0.623  | -28.279 | 4.894  | 1.00 | 0.00  |
| ATOM | 5361 | N    | GLN | 81 | 4.534  | -29.186 | 6.361  | 1.00 | 40.12 |
| ATOM | 5362 | CA   | GLN | 81 | 5.260  | -29.998 | 7.320  | 1.00 | 41.15 |
| ATOM | 5363 | C    | GLN | 81 | 6.411  | -29.085 | 7.711  | 1.00 | 38.66 |
| ATOM | 5364 | O    | GLN | 81 | 7.523  | -29.186 | 7.188  | 1.00 | 38.98 |
| ATOM | 5365 | CB   | GLN | 81 | 5.780  | -31.290 | 6.673  | 1.00 | 46.02 |
| ATOM | 5366 | CG   | GLN | 81 | 4.691  | -32.311 | 6.309  | 1.00 | 51.19 |
| ATOM | 5367 | CD   | GLN | 81 | 5.234  | -33.723 | 6.062  | 1.00 | 53.98 |
| ATOM | 5368 | OE1  | GLN | 81 | 4.560  | -34.560 | 5.456  | 1.00 | 55.34 |
| ATOM | 5369 | NE2  | GLN | 81 | 6.441  | -33.999 | 6.557  | 1.00 | 55.38 |
| ATOM | 5370 | H    | GLN | 81 | 5.060  | -28.563 | 5.806  | 1.00 | 0.00  |
| ATOM | 5371 | HE21 | GLN | 81 | 6.962  | -33.327 | 7.047  | 1.00 | 0.00  |
| ATOM | 5372 | HE22 | GLN | 81 | 6.750  | -34.911 | 6.389  | 1.00 | 0.00  |
| ATOM | 5373 | N    | LEU | 82 | 6.106  | -28.150 | 8.599  | 1.00 | 34.96 |
| ATOM | 5374 | CA   | LEU | 82 | 7.073  | -27.164 | 9.047  | 1.00 | 31.64 |
| ATOM | 5375 | C    | LEU | 82 | 8.137  | -27.671 | 10.001 | 1.00 | 29.83 |
| ATOM | 5376 | O    | LEU | 82 | 7.853  | -28.393 | 10.952 | 1.00 | 29.20 |
| ATOM | 5377 | CB   | LEU | 82 | 6.339  | -25.961 | 9.630  | 1.00 | 30.36 |
| ATOM | 5378 | CG   | LEU | 82 | 5.488  | -25.260 | 8.570  | 1.00 | 27.84 |
| ATOM | 5379 | CD1  | LEU | 82 | 4.432  | -24.393 | 9.210  | 1.00 | 27.47 |
| ATOM | 5380 | CD2  | LEU | 82 | 6.392  | -24.462 | 7.651  | 1.00 | 28.20 |
| ATOM | 5381 | H    | LEU | 82 | 5.216  | -28.133 | 8.998  | 1.00 | 0.00  |
| ATOM | 5382 | N    | LEU | 83 | 9.371  | -27.288 | 9.702  | 1.00 | 29.17 |
| ATOM | 5383 | CA   | LEU | 83 | 10.540 | -27.649 | 10.480 | 1.00 | 28.83 |
| ATOM | 5384 | C    | LEU | 83 | 11.067 | -26.383 | 11.142 | 1.00 | 28.88 |
| ATOM | 5385 | O    | LEU | 83 | 10.995 | -25.303 | 10.565 | 1.00 | 28.95 |
| ATOM | 5386 | CB   | LEU | 83 | 11.612 | -28.208 | 9.546  | 1.00 | 28.59 |
| ATOM | 5387 | CG   | LEU | 83 | 11.178 | -29.387 | 8.675  | 1.00 | 29.06 |
| ATOM | 5388 | CD1  | LEU | 83 | 12.237 | -29.709 | 7.629  | 1.00 | 27.57 |
| ATOM | 5389 | CD2  | LEU | 83 | 10.911 | -30.592 | 9.567  | 1.00 | 30.79 |
| ATOM | 5390 | H    | LEU | 83 | 9.524  | -26.778 | 8.887  | 1.00 | 0.00  |
| ATOM | 5391 | N    | PRO | 84 | 11.527 | -26.486 | 12.390 | 1.00 | 28.99 |
| ATOM | 5392 | CA   | PRO | 84 | 12.063 | -25.334 | 13.121 | 1.00 | 28.88 |
| ATOM | 5393 | C    | PRO | 84 | 13.518 | -25.122 | 12.733 | 1.00 | 28.83 |
| ATOM | 5394 | O    | PRO | 84 | 14.154 | -26.032 | 12.202 | 1.00 | 28.32 |
| ATOM | 5395 | CB   | PRO | 84 | 11.963 | -25.781 | 14.582 | 1.00 | 29.96 |
| ATOM | 5396 | CG   | PRO | 84 | 10.934 | -26.880 | 14.556 | 1.00 | 30.52 |
| ATOM | 5397 | CD   | PRO | 84 | 11.294 | -27.609 | 13.305 | 1.00 | 29.53 |
| ATOM | 5398 | N    | VAL | 85 | 14.047 | -23.936 | 13.008 | 1.00 | 29.60 |

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|------|------|-----|-----|----|--------|---------|--------|------|-------|
| ATOM | 5399 | CA  | VAL | 85 | 15.434 | -23.637 | 12.684 | 1.00 | 30.40 |
| ATOM | 5400 | C   | VAL | 85 | 16.223 | -23.578 | 13.980 | 1.00 | 32.56 |
| ATOM | 5401 | O   | VAL | 85 | 15.781 | -22.950 | 14.939 | 1.00 | 33.84 |
| ATOM | 5402 | CB  | VAL | 85 | 15.563 | -22.296 | 11.941 | 1.00 | 29.41 |
| ATOM | 5403 | CG1 | VAL | 85 | 17.017 | -22.004 | 11.623 | 1.00 | 29.14 |
| ATOM | 5404 | CG2 | VAL | 85 | 14.767 | -22.339 | 10.660 | 1.00 | 29.48 |
| ATOM | 5405 | H   | VAL | 85 | 13.551 | -23.237 | 13.476 | 1.00 | 0.00  |
| ATOM | 5406 | N   | SER | 86 | 17.366 | -24.255 | 14.011 | 1.00 | 34.51 |
| ATOM | 5407 | CA  | SER | 86 | 18.223 | -24.287 | 15.192 | 1.00 | 36.67 |
| ATOM | 5408 | C   | SER | 86 | 19.255 | -23.168 | 15.204 | 1.00 | 38.81 |
| ATOM | 5409 | O   | SER | 86 | 19.760 | -22.803 | 16.269 | 1.00 | 40.54 |
| ATOM | 5410 | CB  | SER | 86 | 18.952 | -25.632 | 15.308 | 1.00 | 36.19 |
| ATOM | 5411 | OG  | SER | 86 | 19.754 | -25.885 | 14.166 | 1.00 | 35.63 |
| ATOM | 5412 | H   | SER | 86 | 17.684 | -24.736 | 13.232 | 1.00 | 0.00  |
| ATOM | 5413 | HG  | SER | 86 | 20.533 | -26.431 | 14.359 | 1.00 | 0.00  |
| ATOM | 5414 | N   | ARG | 87 | 19.567 | -22.614 | 14.035 | 1.00 | 39.15 |
| ATOM | 5415 | CA  | ARG | 87 | 20.570 | -21.557 | 13.972 | 1.00 | 39.04 |
| ATOM | 5416 | C   | ARG | 87 | 20.505 | -20.751 | 12.675 | 1.00 | 36.67 |
| ATOM | 5417 | O   | ARG | 87 | 20.151 | -21.285 | 11.629 | 1.00 | 37.84 |
| ATOM | 5418 | CB  | ARG | 87 | 21.951 | -22.195 | 14.146 | 1.00 | 41.86 |
| ATOM | 5419 | CG  | ARG | 87 | 23.109 | -21.237 | 14.314 | 1.00 | 47.25 |
| ATOM | 5420 | CD  | ARG | 87 | 24.276 | -21.931 | 15.009 | 1.00 | 50.76 |
| ATOM | 5421 | NE  | ARG | 87 | 24.498 | -23.287 | 14.504 | 1.00 | 54.49 |
| ATOM | 5422 | CZ  | ARG | 87 | 25.670 | -23.749 | 14.072 | 1.00 | 56.55 |
| ATOM | 5423 | NH1 | ARG | 87 | 26.747 | -22.965 | 14.078 | 1.00 | 56.52 |
| ATOM | 5424 | NH2 | ARG | 87 | 25.764 | -25.000 | 13.633 | 1.00 | 57.67 |
| ATOM | 5425 | H   | ARG | 87 | 19.150 | -22.963 | 13.217 | 1.00 | 0.00  |
| ATOM | 5426 | HE  | ARG | 87 | 23.732 | -23.924 | 14.491 | 1.00 | 0.00  |
| ATOM | 5427 | HH1 | ARG | 87 | 26.662 | -22.022 | 14.413 | 1.00 | 0.00  |
| ATOM | 5428 | HH2 | ARG | 87 | 27.641 | -23.278 | 13.760 | 1.00 | 0.00  |
| ATOM | 5429 | HH3 | ARG | 87 | 24.928 | -25.593 | 13.624 | 1.00 | 0.00  |
| ATOM | 5430 | HH4 | ARG | 87 | 26.576 | -25.450 | 13.271 | 1.00 | 0.00  |
| ATOM | 5431 | N   | ILE | 88 | 20.818 | -19.460 | 12.754 | 1.00 | 32.92 |
| ATOM | 5432 | CA  | ILE | 88 | 20.812 | -18.584 | 11.587 | 1.00 | 30.06 |
| ATOM | 5433 | C   | ILE | 88 | 22.189 | -17.935 | 11.457 | 1.00 | 29.04 |
| ATOM | 5434 | O   | ILE | 88 | 22.618 | -17.168 | 12.324 | 1.00 | 29.52 |
| ATOM | 5435 | CB  | ILE | 88 | 19.724 | -17.484 | 11.695 | 1.00 | 29.11 |
| ATOM | 5436 | CG1 | ILE | 88 | 18.335 | -18.121 | 11.747 | 1.00 | 28.92 |
| ATOM | 5437 | CG2 | ILE | 88 | 19.796 | -16.546 | 10.499 | 1.00 | 29.01 |
| ATOM | 5438 | H   | ILE | 88 | 21.095 | -19.067 | 13.607 | 1.00 | 0.00  |
| ATOM | 5439 | CD  | ILE | 88 | 17.209 | -17.128 | 11.905 | 1.00 | 28.54 |
| ATOM | 5440 | N   | ILE | 89 | 22.896 | -18.276 | 10.388 | 1.00 | 26.85 |
| ATOM | 5441 | CA  | ILE | 89 | 24.223 | -17.740 | 10.146 | 1.00 | 25.46 |
| ATOM | 5442 | C   | ILE | 89 | 24.246 | -16.855 | 8.895  | 1.00 | 25.86 |
| ATOM | 5443 | O   | ILE | 89 | 24.178 | -17.351 | 7.768  | 1.00 | 25.03 |
| ATOM | 5444 | CB  | ILE | 89 | 25.237 | -18.882 | 9.985  | 1.00 | 24.73 |
| ATOM | 5445 | CG1 | ILE | 89 | 25.132 | -19.835 | 11.169 | 1.00 | 23.29 |
| ATOM | 5446 | CG2 | ILE | 89 | 26.652 | -18.336 | 9.899  | 1.00 | 25.35 |
| ATOM | 5447 | H   | ILE | 89 | 22.536 | -18.911 | 9.737  | 1.00 | 0.00  |
| ATOM | 5448 | CD  | ILE | 89 | 26.061 | -20.988 | 11.069 | 1.00 | 23.27 |
| ATOM | 5449 | N   | VAL | 90 | 24.285 | -15.543 | 9.108  | 1.00 | 25.60 |
| ATOM | 5450 | CA  | VAL | 90 | 24.333 | -14.570 | 8.019  | 1.00 | 25.27 |
| ATOM | 5451 | C   | VAL | 90 | 25.803 | -14.232 | 7.783  | 1.00 | 26.43 |
| ATOM | 5452 | O   | VAL | 90 | 26.621 | -14.381 | 8.692  | 1.00 | 28.33 |
| ATOM | 5453 | CB  | VAL | 90 | 23.558 | -13.273 | 8.397  | 1.00 | 24.27 |
| ATOM | 5454 | CG1 | VAL | 90 | 23.860 | -12.148 | 7.417  | 1.00 | 23.87 |
| ATOM | 5455 | CG2 | VAL | 90 | 22.067 | -13.543 | 8.404  | 1.00 | 24.36 |
| ATOM | 5456 | H   | VAL | 90 | 24.307 | -15.220 | 10.030 | 1.00 | 0.00  |
| ATOM | 5457 | N   | HIS | 91 | 26.158 | -13.828 | 6.564  | 1.00 | 25.18 |
| ATOM | 5458 | CA  | HIS | 91 | 27.538 | -13.461 | 6.291  | 1.00 | 23.69 |
| ATOM | 5459 | C   | HIS | 91 | 27.865 | -12.134 | 6.968  | 1.00 | 25.88 |
| ATOM | 5460 | O   | HIS | 91 | 27.150 | -11.152 | 6.806  | 1.00 | 27.46 |
| ATOM | 5461 | CB  | HIS | 91 | 27.792 | -13.344 | 4.797  | 1.00 | 20.41 |

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|      |      |      |     |    |        |         |       |      |       |
|------|------|------|-----|----|--------|---------|-------|------|-------|
| ATOM | 5462 | CG   | HIS | 91 | 29.244 | -13.303 | 4.450 | 1.00 | 17.87 |
| ATOM | 5463 | ND1  | HIS | 91 | 29.941 | -14.416 | 4.037 | 1.00 | 17.67 |
| ATOM | 5464 | CD2  | HIS | 91 | 30.144 | -12.293 | 4.491 | 1.00 | 17.69 |
| ATOM | 5465 | CE1  | HIS | 91 | 31.205 | -14.097 | 3.836 | 1.00 | 16.11 |
| ATOM | 5466 | NE2  | HIS | 91 | 31.355 | -12.815 | 4.106 | 1.00 | 17.58 |
| ATOM | 5467 | H    | HIS | 91 | 25.502 | -13.828 | 5.836 | 1.00 | 0.00  |
| ATOM | 5468 | HD1  | HIS | 91 | 29.559 | -15.316 | 3.916 | 1.00 | 0.00  |
| ATOM | 5469 | HE2  | HIS | 91 | 32.231 | -12.350 | 4.057 | 1.00 | 0.00  |
| ATOM | 5470 | N    | PRO | 92 | 28.983 | -12.081 | 7.703 | 1.00 | 27.94 |
| ATOM | 5471 | CA   | PRO | 92 | 29.476 | -10.907 | 8.436 | 1.00 | 27.75 |
| ATOM | 5472 | C    | PRO | 92 | 29.511 | -9.569  | 7.692 | 1.00 | 27.23 |
| ATOM | 5473 | O    | PRO | 92 | 29.109 | -8.547  | 8.234 | 1.00 | 26.38 |
| ATOM | 5474 | CB   | PRO | 92 | 30.881 | -11.342 | 8.842 | 1.00 | 28.69 |
| ATOM | 5475 | CG   | PRO | 92 | 30.688 | -12.798 | 9.123 | 1.00 | 29.76 |
| ATOM | 5476 | CD   | PRO | 92 | 29.848 | -13.251 | 7.951 | 1.00 | 29.47 |
| ATOM | 5477 | N    | GLN | 93 | 30.013 | -9.569  | 6.465 | 1.00 | 28.86 |
| ATOM | 5478 | CA   | GLN | 93 | 30.124 | -8.335  | 5.686 | 1.00 | 29.95 |
| ATOM | 5479 | C    | GLN | 93 | 28.828 | -7.875  | 5.050 | 1.00 | 27.27 |
| ATOM | 5480 | O    | GLN | 93 | 28.832 | -6.989  | 4.202 | 1.00 | 27.53 |
| ATOM | 5481 | CB   | GLN | 93 | 31.193 | -8.493  | 4.599 | 1.00 | 34.89 |
| ATOM | 5482 | CG   | GLN | 93 | 32.615 | -8.664  | 5.129 | 1.00 | 40.63 |
| ATOM | 5483 | CD   | GLN | 93 | 33.482 | -9.485  | 4.187 | 1.00 | 44.77 |
| ATOM | 5484 | OE1  | GLN | 93 | 33.863 | -10.617 | 4.504 | 1.00 | 47.44 |
| ATOM | 5485 | NE2  | GLN | 93 | 33.750 | -8.945  | 3.004 | 1.00 | 46.56 |
| ATOM | 5486 | H    | GLN | 93 | 30.325 | -10.403 | 6.086 | 1.00 | 0.00  |
| ATOM | 5487 | HE21 | GLN | 93 | 33.374 | -8.067  | 2.790 | 1.00 | 0.00  |
| ATOM | 5488 | HE22 | GLN | 93 | 34.338 | -9.464  | 2.415 | 1.00 | 0.00  |
| ATOM | 5489 | N    | PHE | 94 | 27.719 | -8.465  | 5.462 | 1.00 | 25.36 |
| ATOM | 5490 | CA   | PHE | 94 | 26.439 | -8.103  | 4.892 | 1.00 | 23.30 |
| ATOM | 5491 | C    | PHE | 94 | 25.658 | -7.043  | 5.642 | 1.00 | 23.06 |
| ATOM | 5492 | O    | PHE | 94 | 25.521 | -7.097  | 6.859 | 1.00 | 22.78 |
| ATOM | 5493 | CB   | PHE | 94 | 25.553 | -9.337  | 4.733 | 1.00 | 22.18 |
| ATOM | 5494 | CG   | PHE | 94 | 24.148 | -9.015  | 4.304 | 1.00 | 22.62 |
| ATOM | 5495 | CD1  | PHE | 94 | 23.863 | -8.710  | 2.976 | 1.00 | 23.07 |
| ATOM | 5496 | CD2  | PHE | 94 | 23.115 | -8.981  | 5.234 | 1.00 | 22.45 |
| ATOM | 5497 | CE1  | PHE | 94 | 22.576 | -8.372  | 2.582 | 1.00 | 21.22 |
| ATOM | 5498 | CE2  | PHE | 94 | 21.827 | -8.646  | 4.848 | 1.00 | 21.68 |
| ATOM | 5499 | CZ   | PHE | 94 | 21.558 | -8.341  | 3.519 | 1.00 | 21.64 |
| ATOM | 5500 | H    | PHE | 94 | 27.686 | -9.148  | 6.159 | 1.00 | 0.00  |
| ATOM | 5501 | N    | TYR | 95 | 25.123 | -6.091  | 4.883 | 1.00 | 22.81 |
| ATOM | 5502 | CA   | TYR | 95 | 24.280 | -5.038  | 5.427 | 1.00 | 20.65 |
| ATOM | 5503 | C    | TYR | 95 | 23.194 | -4.679  | 4.417 | 1.00 | 20.98 |
| ATOM | 5504 | O    | TYR | 95 | 22.070 | -4.338  | 4.803 | 1.00 | 21.34 |
| ATOM | 5505 | CB   | TYR | 95 | 25.068 | -3.777  | 5.788 | 1.00 | 19.90 |
| ATOM | 5506 | CG   | TYR | 95 | 24.149 | -2.719  | 6.355 | 1.00 | 18.68 |
| ATOM | 5507 | CD1  | TYR | 95 | 23.578 | -2.873  | 7.622 | 1.00 | 19.10 |
| ATOM | 5508 | CD2  | TYR | 95 | 23.755 | -1.625  | 5.588 | 1.00 | 15.97 |
| ATOM | 5509 | CE1  | TYR | 95 | 22.633 | -1.974  | 8.105 | 1.00 | 18.09 |
| ATOM | 5510 | CE2  | TYR | 95 | 22.814 | -0.723  | 6.059 | 1.00 | 16.50 |
| ATOM | 5511 | CZ   | TYR | 95 | 22.254 | -0.900  | 7.316 | 1.00 | 18.07 |
| ATOM | 5512 | OH   | TYR | 95 | 21.315 | -0.005  | 7.782 | 1.00 | 18.55 |
| ATOM | 5513 | H    | TYR | 95 | 25.344 | -6.145  | 3.934 | 1.00 | 0.00  |
| ATOM | 5514 | HH   | TYR | 95 | 20.866 | -0.394  | 8.555 | 1.00 | 0.00  |
| ATOM | 5515 | N    | THR | 96 | 23.521 | -4.819  | 3.131 | 1.00 | 21.44 |
| ATOM | 5516 | CA   | THR | 96 | 22.618 | -4.484  | 2.028 | 1.00 | 21.14 |
| ATOM | 5517 | C    | THR | 96 | 22.903 | -5.343  | 0.792 | 1.00 | 21.90 |
| ATOM | 5518 | O    | THR | 96 | 24.062 | -5.616  | 0.484 | 1.00 | 23.14 |
| ATOM | 5519 | CB   | THR | 96 | 22.799 | -3.001  | 1.646 | 1.00 | 20.72 |
| ATOM | 5520 | OG1  | THR | 96 | 22.102 | -2.170  | 2.579 | 1.00 | 20.25 |
| ATOM | 5521 | CG2  | THR | 96 | 22.309 | -2.739  | 0.262 | 1.00 | 21.80 |
| ATOM | 5522 | H    | THR | 96 | 24.396 | -5.168  | 2.868 | 1.00 | 0.00  |
| ATOM | 5523 | HG1  | THR | 96 | 22.131 | -1.265  | 2.253 | 1.00 | 0.00  |
| ATOM | 5524 | N    | ALA | 97 | 21.850 | -5.711  | 0.059 | 1.00 | 22.79 |

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|      |      |      |     |     |        |         |        |      |       |
|------|------|------|-----|-----|--------|---------|--------|------|-------|
| ATOM | 5525 | CA   | ALA | 97  | 21.972 | -6.536  | -1.153 | 1.00 | 22.89 |
| ATOM | 5526 | C    | ALA | 97  | 22.844 | -5.864  | -2.209 | 1.00 | 24.01 |
| ATOM | 5527 | O    | ALA | 97  | 23.755 | -6.478  | -2.770 | 1.00 | 23.73 |
| ATOM | 5528 | CB   | ALA | 97  | 20.591 | -6.823  | -1.737 | 1.00 | 20.14 |
| ATOM | 5529 | H    | ALA | 97  | 20.967 | -5.419  | 0.359  | 1.00 | 0.00  |
| ATOM | 5530 | N    | GLN | 98  | 22.580 | -4.579  | -2.434 | 1.00 | 24.56 |
| ATOM | 5531 | CA   | GLN | 98  | 23.305 | -3.788  | -3.425 | 1.00 | 23.73 |
| ATOM | 5532 | C    | GLN | 98  | 24.787 | -3.690  | -3.110 | 1.00 | 23.19 |
| ATOM | 5533 | O    | GLN | 98  | 25.623 | -3.622  | -4.007 | 1.00 | 23.76 |
| ATOM | 5534 | CB   | GLN | 98  | 22.701 | -2.386  | -3.534 | 1.00 | 23.17 |
| ATOM | 5535 | CG   | GLN | 98  | 21.249 | -2.349  | -4.013 | 1.00 | 23.51 |
| ATOM | 5536 | CD   | GLN | 98  | 20.275 | -2.957  | -3.017 | 1.00 | 23.26 |
| ATOM | 5537 | OE1  | GLN | 98  | 20.129 | -2.471  | -1.900 | 1.00 | 23.95 |
| ATOM | 5538 | NE2  | GLN | 98  | 19.622 | -4.037  | -3.408 | 1.00 | 23.99 |
| ATOM | 5539 | H    | GLN | 98  | 21.904 | -4.150  | -1.877 | 1.00 | 0.00  |
| ATOM | 5540 | HE21 | GLN | 98  | 19.794 | -4.391  | -4.306 | 1.00 | 0.00  |
| ATOM | 5541 | HE22 | GLN | 98  | 18.971 | -4.433  | -2.791 | 1.00 | 0.00  |
| ATOM | 5542 | N    | ILE | 99  | 25.110 | -3.663  | -1.827 | 1.00 | 23.76 |
| ATOM | 5543 | CA   | ILE | 99  | 26.496 | -3.575  | -1.407 | 1.00 | 24.99 |
| ATOM | 5544 | C    | ILE | 99  | 27.202 | -4.907  | -1.616 | 1.00 | 25.61 |
| ATOM | 5545 | O    | ILE | 99  | 28.359 | -4.934  | -2.035 | 1.00 | 27.44 |
| ATOM | 5546 | CB   | ILE | 99  | 26.607 | -3.128  | 0.055  | 1.00 | 25.61 |
| ATOM | 5547 | CG1  | ILE | 99  | 26.091 | -1.690  | 0.192  | 1.00 | 26.26 |
| ATOM | 5548 | CG2  | ILE | 99  | 28.041 | -3.229  | 0.519  | 1.00 | 26.62 |
| ATOM | 5549 | H    | ILE | 99  | 24.412 | -3.721  | -1.153 | 1.00 | 0.00  |
| ATOM | 5550 | CD   | ILE | 99  | 26.142 | -1.131  | 1.596  | 1.00 | 25.64 |
| ATOM | 5551 | N    | GLY | 100 | 26.515 | -6.006  | -1.315 | 1.00 | 25.29 |
| ATOM | 5552 | CA   | GLY | 100 | 27.100 | -7.322  | -1.509 | 1.00 | 23.95 |
| ATOM | 5553 | C    | GLY | 100 | 27.054 | -8.204  | -0.276 | 1.00 | 23.20 |
| ATOM | 5554 | O    | GLY | 100 | 26.540 | -7.784  | 0.767  | 1.00 | 22.23 |
| ATOM | 5555 | H    | GLY | 100 | 25.643 | -5.948  | -0.876 | 1.00 | 0.00  |
| ATOM | 5556 | N    | ALA | 101 | 27.595 | -9.420  | -0.402 | 1.00 | 22.09 |
| ATOM | 5557 | CA   | ALA | 101 | 27.645 | -10.397 | 0.683  | 1.00 | 20.59 |
| ATOM | 5558 | C    | ALA | 101 | 26.260 | -10.844 | 1.123  | 1.00 | 20.34 |
| ATOM | 5559 | O    | ALA | 101 | 26.012 | -11.078 | 2.310  | 1.00 | 21.30 |
| ATOM | 5560 | CB   | ALA | 101 | 28.429 | -9.838  | 1.873  | 1.00 | 20.59 |
| ATOM | 5561 | H    | ALA | 101 | 28.019 | -9.686  | -1.261 | 1.00 | 0.00  |
| ATOM | 5562 | N    | ASP | 102 | 25.368 | -10.999 | 0.156  | 1.00 | 18.24 |
| ATOM | 5563 | CA   | ASP | 102 | 24.005 | -11.418 | 0.439  | 1.00 | 16.15 |
| ATOM | 5564 | C    | ASP | 102 | 23.897 | -12.933 | 0.428  | 1.00 | 16.12 |
| ATOM | 5565 | O    | ASP | 102 | 23.564 | -13.529 | -0.599 | 1.00 | 15.74 |
| ATOM | 5566 | CB   | ASP | 102 | 23.069 | -10.844 | -0.613 | 1.00 | 15.16 |
| ATOM | 5567 | CG   | ASP | 102 | 21.626 | -10.942 | -0.222 | 1.00 | 14.32 |
| ATOM | 5568 | OD1  | ASP | 102 | 21.291 | -11.656 | 0.738  | 1.00 | 13.59 |
| ATOM | 5569 | OD2  | ASP | 102 | 20.802 | -10.275 | -0.870 | 1.00 | 16.56 |
| ATOM | 5570 | H    | ASP | 102 | 25.639 | -10.827 | -0.768 | 1.00 | 0.00  |
| ATOM | 5571 | N    | ILE | 103 | 24.188 | -13.559 | 1.563  | 1.00 | 15.23 |
| ATOM | 5572 | CA   | ILE | 103 | 24.113 | -15.012 | 1.668  | 1.00 | 14.17 |
| ATOM | 5573 | C    | ILE | 103 | 24.041 | -15.431 | 3.128  | 1.00 | 15.92 |
| ATOM | 5574 | O    | ILE | 103 | 24.574 | -14.741 | 4.004  | 1.00 | 17.27 |
| ATOM | 5575 | CB   | ILE | 103 | 25.318 | -15.700 | 0.976  | 1.00 | 11.92 |
| ATOM | 5576 | CG1  | ILE | 103 | 25.110 | -17.218 | 0.954  | 1.00 | 11.52 |
| ATOM | 5577 | CG2  | ILE | 103 | 26.614 | -15.335 | 1.667  | 1.00 | 8.11  |
| ATOM | 5578 | H    | ILE | 103 | 24.452 | -13.034 | 2.349  | 1.00 | 0.00  |
| ATOM | 5579 | CD   | ILE | 103 | 26.013 | -17.957 | -0.004 | 1.00 | 8.58  |
| ATOM | 5580 | N    | ALA | 104 | 23.360 | -16.544 | 3.391  | 1.00 | 16.74 |
| ATOM | 5581 | CA   | ALA | 104 | 23.208 | -17.050 | 4.749  | 1.00 | 17.15 |
| ATOM | 5582 | C    | ALA | 104 | 22.887 | -18.544 | 4.781  | 1.00 | 18.33 |
| ATOM | 5583 | O    | ALA | 104 | 22.475 | -19.134 | 3.773  | 1.00 | 17.78 |
| ATOM | 5584 | CB   | ALA | 104 | 22.130 | -16.263 | 5.483  | 1.00 | 15.16 |
| ATOM | 5585 | H    | ALA | 104 | 22.928 | -17.049 | 2.677  | 1.00 | 0.00  |
| ATOM | 5586 | N    | LEU | 105 | 23.106 | -19.143 | 5.947  | 1.00 | 20.15 |
| ATOM | 5587 | CA   | LEU | 105 | 22.857 | -20.563 | 6.186  | 1.00 | 21.24 |

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|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 5588 | C   | LEU | 105 | 21.902 | -20.733 | 7.363  | 1.00 | 22.18 |
| ATOM | 5589 | O   | LEU | 105 | 22.102 | -20.144 | 8.426  | 1.00 | 22.09 |
| ATOM | 5590 | CB  | LEU | 105 | 24.164 | -21.283 | 6.520  | 1.00 | 19.66 |
| ATOM | 5591 | CG  | LEU | 105 | 25.216 | -21.373 | 5.428  | 1.00 | 18.88 |
| ATOM | 5592 | CD1 | LEU | 105 | 26.535 | -21.826 | 6.025  | 1.00 | 19.97 |
| ATOM | 5593 | CD2 | LEU | 105 | 24.739 | -22.326 | 4.350  | 1.00 | 19.61 |
| ATOM | 5594 | H   | LEU | 105 | 23.461 | -18.600 | 6.670  | 1.00 | 0.00  |
| ATOM | 5595 | N   | LEU | 106 | 20.855 | -21.522 | 7.161  | 1.00 | 23.24 |
| ATOM | 5596 | CA  | LEU | 106 | 19.883 | -21.789 | 8.209  | 1.00 | 24.80 |
| ATOM | 5597 | C   | LEU | 106 | 20.140 | -23.222 | 8.659  | 1.00 | 27.36 |
| ATOM | 5598 | O   | LEU | 106 | 20.129 | -24.135 | 7.829  | 1.00 | 29.36 |
| ATOM | 5599 | CB  | LEU | 106 | 18.452 | -21.682 | 7.662  | 1.00 | 22.40 |
| ATOM | 5600 | CG  | LEU | 106 | 17.949 | -20.421 | 6.945  | 1.00 | 19.82 |
| ATOM | 5601 | CD1 | LEU | 106 | 16.500 | -20.643 | 6.572  | 1.00 | 18.52 |
| ATOM | 5602 | CD2 | LEU | 106 | 18.070 | -19.181 | 7.813  | 1.00 | 19.34 |
| ATOM | 5603 | H   | LEU | 106 | 20.752 | -21.927 | 6.289  | 1.00 | 0.00  |
| ATOM | 5604 | N   | GLU | 107 | 20.444 | -23.425 | 9.935  | 1.00 | 28.30 |
| ATOM | 5605 | CA  | GLU | 107 | 20.671 | -24.777 | 10.415 | 1.00 | 30.97 |
| ATOM | 5606 | C   | GLU | 107 | 19.374 | -25.338 | 10.954 | 1.00 | 31.56 |
| ATOM | 5607 | O   | GLU | 107 | 18.707 | -24.696 | 11.755 | 1.00 | 32.38 |
| ATOM | 5608 | CB  | GLU | 107 | 21.730 | -24.833 | 11.509 | 1.00 | 33.24 |
| ATOM | 5609 | CG  | GLU | 107 | 21.909 | -26.249 | 12.043 | 1.00 | 36.31 |
| ATOM | 5610 | CD  | GLU | 107 | 23.049 | -26.377 | 13.012 | 1.00 | 38.81 |
| ATOM | 5611 | OE1 | GLU | 107 | 24.070 | -26.995 | 12.643 | 1.00 | 40.32 |
| ATOM | 5612 | OE2 | GLU | 107 | 22.948 | -25.852 | 14.143 | 1.00 | 40.95 |
| ATOM | 5613 | H   | GLU | 107 | 20.472 | -22.672 | 10.541 | 1.00 | 0.00  |
| ATOM | 5614 | N   | LEU | 108 | 19.017 | -26.530 | 10.503 | 1.00 | 31.89 |
| ATOM | 5615 | CA  | LEU | 108 | 17.799 | -27.180 | 10.942 | 1.00 | 34.62 |
| ATOM | 5616 | C   | LEU | 108 | 18.095 | -27.931 | 12.228 | 1.00 | 38.46 |
| ATOM | 5617 | O   | LEU | 108 | 19.217 | -28.384 | 12.432 | 1.00 | 39.52 |
| ATOM | 5618 | CB  | LEU | 108 | 17.316 | -28.150 | 9.864  | 1.00 | 33.85 |
| ATOM | 5619 | CG  | LEU | 108 | 17.126 | -27.540 | 8.473  | 1.00 | 32.27 |
| ATOM | 5620 | CD1 | LEU | 108 | 16.728 | -28.611 | 7.467  | 1.00 | 30.91 |
| ATOM | 5621 | CD2 | LEU | 108 | 16.071 | -26.451 | 8.543  | 1.00 | 31.50 |
| ATOM | 5622 | H   | LEU | 108 | 19.626 | -26.977 | 9.894  | 1.00 | 0.00  |
| ATOM | 5623 | N   | GLU | 109 | 17.090 | -28.076 | 13.087 | 1.00 | 42.87 |
| ATOM | 5624 | CA  | GLU | 109 | 17.258 | -28.785 | 14.360 | 1.00 | 47.08 |
| ATOM | 5625 | C   | GLU | 109 | 17.692 | -30.240 | 14.187 | 1.00 | 50.76 |
| ATOM | 5626 | O   | GLU | 109 | 18.284 | -30.832 | 15.100 | 1.00 | 52.06 |
| ATOM | 5627 | CB  | GLU | 109 | 15.966 | -28.753 | 15.184 | 1.00 | 46.61 |
| ATOM | 5628 | CG  | GLU | 109 | 15.781 | -27.525 | 16.068 | 1.00 | 47.13 |
| ATOM | 5629 | CD  | GLU | 109 | 14.501 | -27.583 | 16.906 | 1.00 | 47.76 |
| ATOM | 5630 | OE1 | GLU | 109 | 14.123 | -26.537 | 17.473 | 1.00 | 47.83 |
| ATOM | 5631 | OE2 | GLU | 109 | 13.866 | -28.660 | 16.998 | 1.00 | 47.19 |
| ATOM | 5632 | H   | GLU | 109 | 16.213 | -27.699 | 12.866 | 1.00 | 0.00  |
| ATOM | 5633 | N   | GLU | 110 | 17.404 | -30.815 | 13.020 | 1.00 | 52.59 |
| ATOM | 5634 | CA  | GLU | 110 | 17.756 | -32.203 | 12.759 | 1.00 | 53.86 |
| ATOM | 5635 | C   | GLU | 110 | 17.811 | -32.464 | 11.261 | 1.00 | 53.25 |
| ATOM | 5636 | O   | GLU | 110 | 17.112 | -31.803 | 10.491 | 1.00 | 53.33 |
| ATOM | 5637 | CB  | GLU | 110 | 16.714 | -33.126 | 13.387 | 1.00 | 56.53 |
| ATOM | 5638 | CG  | GLU | 110 | 17.275 | -34.465 | 13.822 | 1.00 | 60.87 |
| ATOM | 5639 | CD  | GLU | 110 | 16.246 | -35.575 | 13.815 | 1.00 | 63.05 |
| ATOM | 5640 | OE1 | GLU | 110 | 15.031 | -35.271 | 13.857 | 1.00 | 64.92 |
| ATOM | 5641 | OE2 | GLU | 110 | 16.664 | -36.755 | 13.769 | 1.00 | 63.74 |
| ATOM | 5642 | H   | GLU | 110 | 16.967 | -30.311 | 12.304 | 1.00 | 0.00  |
| ATOM | 5643 | N   | PRO | 111 | 18.668 | -33.404 | 10.827 | 1.00 | 52.58 |
| ATOM | 5644 | CA  | PRO | 111 | 18.803 | -33.739 | 9.408  | 1.00 | 52.57 |
| ATOM | 5645 | C   | PRO | 111 | 17.571 | -34.420 | 8.831  | 1.00 | 52.09 |
| ATOM | 5646 | O   | PRO | 111 | 16.993 | -35.309 | 9.449  | 1.00 | 52.64 |
| ATOM | 5647 | CB  | PRO | 111 | 20.016 | -34.672 | 9.391  | 1.00 | 52.54 |
| ATOM | 5648 | CG  | PRO | 111 | 19.971 | -35.311 | 10.732 | 1.00 | 52.26 |
| ATOM | 5649 | CD  | PRO | 111 | 19.669 | -34.135 | 11.621 | 1.00 | 52.48 |
| ATOM | 5650 | N   | VAL | 112 | 17.165 | -33.972 | 7.651  | 1.00 | 51.73 |

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|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 5651 | CA  | VAL | 112 | 16.011 | -34.524 | 6.959  | 1.00 | 51.86 |
| ATOM | 5652 | C   | VAL | 112 | 16.417 | -35.861 | 6.363  | 1.00 | 53.40 |
| ATOM | 5653 | O   | VAL | 112 | 17.596 | -36.083 | 6.087  | 1.00 | 54.58 |
| ATOM | 5654 | CB  | VAL | 112 | 15.558 | -33.599 | 5.804  | 1.00 | 50.44 |
| ATOM | 5655 | CG1 | VAL | 112 | 15.323 | -32.192 | 6.315  | 1.00 | 49.69 |
| ATOM | 5656 | CG2 | VAL | 112 | 16.589 | -33.595 | 4.682  | 1.00 | 49.08 |
| ATOM | 5657 | H   | VAL | 112 | 17.664 | -33.234 | 7.269  | 1.00 | 0.00  |
| ATOM | 5658 | N   | LYS | 113 | 15.449 | -36.749 | 6.154  | 1.00 | 54.48 |
| ATOM | 5659 | CA  | LYS | 113 | 15.752 | -38.044 | 5.559  | 1.00 | 55.92 |
| ATOM | 5660 | C   | LYS | 113 | 15.645 | -37.879 | 4.040  | 1.00 | 56.43 |
| ATOM | 5661 | O   | LYS | 113 | 14.581 | -38.065 | 3.442  | 1.00 | 55.93 |
| ATOM | 5662 | CB  | LYS | 113 | 14.805 | -39.129 | 6.094  | 1.00 | 56.81 |
| ATOM | 5663 | CG  | LYS | 113 | 15.481 | -40.490 | 6.286  | 1.00 | 56.61 |
| ATOM | 5664 | CD  | LYS | 113 | 14.673 | -41.410 | 7.193  | 1.00 | 55.90 |
| ATOM | 5665 | CE  | LYS | 113 | 15.441 | -42.687 | 7.520  | 1.00 | 55.73 |
| ATOM | 5666 | NZ  | LYS | 113 | 15.661 | -43.558 | 6.330  | 1.00 | 55.26 |
| ATOM | 5667 | H   | LYS | 113 | 14.523 | -36.532 | 6.380  | 1.00 | 0.00  |
| ATOM | 5668 | HZ1 | LYS | 113 | 16.157 | -43.039 | 5.576  | 1.00 | 0.00  |
| ATOM | 5669 | HZ2 | LYS | 113 | 14.734 | -43.872 | 5.974  | 1.00 | 0.00  |
| ATOM | 5670 | HZ3 | LYS | 113 | 16.218 | -44.390 | 6.611  | 1.00 | 0.00  |
| ATOM | 5671 | N   | VAL | 114 | 16.763 | -37.471 | 3.446  | 1.00 | 58.00 |
| ATOM | 5672 | CA  | VAL | 114 | 16.881 | -37.216 | 2.012  | 1.00 | 59.49 |
| ATOM | 5673 | C   | VAL | 114 | 16.420 | -38.318 | 1.063  | 1.00 | 59.56 |
| ATOM | 5674 | O   | VAL | 114 | 17.173 | -39.240 | 0.740  | 1.00 | 60.42 |
| ATOM | 5675 | CB  | VAL | 114 | 18.329 | -36.794 | 1.628  | 1.00 | 60.33 |
| ATOM | 5676 | CG1 | VAL | 114 | 18.593 | -35.361 | 2.072  | 1.00 | 61.61 |
| ATOM | 5677 | CG2 | VAL | 114 | 19.350 | -37.737 | 2.260  | 1.00 | 60.64 |
| ATOM | 5678 | H   | VAL | 114 | 17.548 | -37.339 | 4.010  | 1.00 | 0.00  |
| ATOM | 5679 | N   | SER | 115 | 15.180 | -38.203 | 0.602  | 1.00 | 58.74 |
| ATOM | 5680 | CA  | SER | 115 | 14.618 | -39.171 | -0.328 | 1.00 | 57.94 |
| ATOM | 5681 | C   | SER | 115 | 14.887 | -38.683 | -1.753 | 1.00 | 58.30 |
| ATOM | 5682 | O   | SER | 115 | 15.505 | -37.633 | -1.954 | 1.00 | 58.38 |
| ATOM | 5683 | CB  | SER | 115 | 13.109 | -39.301 | -0.097 | 1.00 | 57.48 |
| ATOM | 5684 | OG  | SER | 115 | 12.431 | -38.072 | -0.322 | 1.00 | 56.56 |
| ATOM | 5685 | H   | SER | 115 | 14.663 | -37.426 | 0.901  | 1.00 | 0.00  |
| ATOM | 5686 | HG  | SER | 115 | 12.349 | -37.552 | 0.510  | 1.00 | 0.00  |
| ATOM | 5687 | N   | SER | 116 | 14.414 | -39.426 | -2.748 | 1.00 | 58.64 |
| ATOM | 5688 | CA  | SER | 116 | 14.602 | -39.010 | -4.137 | 1.00 | 58.55 |
| ATOM | 5689 | C   | SER | 116 | 13.640 | -37.867 | -4.453 | 1.00 | 57.96 |
| ATOM | 5690 | O   | SER | 116 | 13.676 | -37.284 | -5.532 | 1.00 | 58.14 |
| ATOM | 5691 | CB  | SER | 116 | 14.353 | -40.179 | -5.095 | 1.00 | 58.97 |
| ATOM | 5692 | OG  | SER | 116 | 14.596 | -39.805 | -6.442 | 1.00 | 59.12 |
| ATOM | 5693 | H   | SER | 116 | 14.003 | -40.296 | -2.564 | 1.00 | 0.00  |
| ATOM | 5694 | HG  | SER | 116 | 14.563 | -40.578 | -7.023 | 1.00 | 0.00  |
| ATOM | 5695 | N   | HIS | 117 | 12.804 | -37.531 | -3.480 | 1.00 | 57.28 |
| ATOM | 5696 | CA  | HIS | 117 | 11.819 | -36.477 | -3.643 | 1.00 | 57.04 |
| ATOM | 5697 | C   | HIS | 117 | 12.306 | -35.227 | -2.929 | 1.00 | 53.82 |
| ATOM | 5698 | O   | HIS | 117 | 11.908 | -34.113 | -3.262 | 1.00 | 53.92 |
| ATOM | 5699 | CB  | HIS | 117 | 10.486 | -36.943 | -3.057 | 1.00 | 61.50 |
| ATOM | 5700 | CG  | HIS | 117 | 10.263 | -38.421 | -3.182 | 1.00 | 65.95 |
| ATOM | 5701 | ND1 | HIS | 117 | 10.494 | -39.115 | -4.353 | 1.00 | 66.97 |
| ATOM | 5702 | CD2 | HIS | 117 | 9.867  | -39.344 | -2.272 | 1.00 | 67.49 |
| ATOM | 5703 | CE1 | HIS | 117 | 10.250 | -40.400 | -4.158 | 1.00 | 67.74 |
| ATOM | 5704 | NE2 | HIS | 117 | 9.868  | -40.565 | -2.904 | 1.00 | 68.34 |
| ATOM | 5705 | H   | HIS | 117 | 12.838 | -37.918 | -2.589 | 1.00 | 0.00  |
| ATOM | 5706 | HD1 | HIS | 117 | 10.768 | -38.712 | -5.215 | 1.00 | 0.00  |
| ATOM | 5707 | HE2 | HIS | 117 | 9.593  | -41.405 | -2.468 | 1.00 | 0.00  |
| ATOM | 5708 | N   | VAL | 118 | 13.153 | -35.422 | -1.927 | 1.00 | 49.78 |
| ATOM | 5709 | CA  | VAL | 118 | 13.701 | -34.311 | -1.171 | 1.00 | 47.22 |
| ATOM | 5710 | C   | VAL | 118 | 15.192 | -34.519 | -0.950 | 1.00 | 46.21 |
| ATOM | 5711 | O   | VAL | 118 | 15.595 | -35.179 | 0.004  | 1.00 | 46.12 |
| ATOM | 5712 | CB  | VAL | 118 | 13.017 | -34.185 | 0.205  | 1.00 | 46.77 |
| ATOM | 5713 | CG1 | VAL | 118 | 13.604 | -33.014 | 0.981  | 1.00 | 47.74 |

|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 5714 | CG2 | VAL | 118 | 11.528 | -34.009 | 0.034  | 1.00 | 47.11 |
| ATOM | 5715 | H   | VAL | 118 | 13.381 | -36.322 | -1.619 | 1.00 | 0.00  |
| ATOM | 5716 | N   | HIS | 119 | 16.018 | -33.979 | -1.836 | 1.00 | 45.58 |
| ATOM | 5717 | CA  | HIS | 119 | 17.453 | -34.132 | -1.669 | 1.00 | 45.66 |
| ATOM | 5718 | C   | HIS | 119 | 18.275 | -32.925 | -2.072 | 1.00 | 45.32 |
| ATOM | 5719 | O   | HIS | 119 | 17.886 | -32.131 | -2.928 | 1.00 | 45.78 |
| ATOM | 5720 | CB  | HIS | 119 | 17.981 | -35.410 | -2.332 | 1.00 | 46.88 |
| ATOM | 5721 | CG  | HIS | 119 | 17.685 | -35.517 | -3.795 | 1.00 | 47.79 |
| ATOM | 5722 | ND1 | HIS | 119 | 16.636 | -36.262 | -4.286 | 1.00 | 48.22 |
| ATOM | 5723 | CD2 | HIS | 119 | 18.325 | -35.010 | -4.877 | 1.00 | 48.49 |
| ATOM | 5724 | CE1 | HIS | 119 | 16.639 | -36.211 | -5.606 | 1.00 | 48.59 |
| ATOM | 5725 | NE2 | HIS | 119 | 17.653 | -35.457 | -5.989 | 1.00 | 49.25 |
| ATOM | 5726 | H   | HIS | 119 | 15.661 | -33.402 | -2.546 | 1.00 | 0.00  |
| ATOM | 5727 | HD1 | HIS | 119 | 16.021 | -36.755 | -3.698 | 1.00 | 0.00  |
| ATOM | 5728 | HE2 | HIS | 119 | 17.881 | -35.229 | -6.917 | 1.00 | 0.00  |
| ATOM | 5729 | N   | THR | 120 | 19.428 | -32.820 | -1.429 | 1.00 | 44.24 |
| ATOM | 5730 | CA  | THR | 120 | 20.371 | -31.734 | -1.613 | 1.00 | 42.99 |
| ATOM | 5731 | C   | THR | 120 | 20.920 | -31.497 | -3.014 | 1.00 | 42.36 |
| ATOM | 5732 | O   | THR | 120 | 21.071 | -32.427 | -3.808 | 1.00 | 42.67 |
| ATOM | 5733 | CB  | THR | 120 | 21.541 | -31.917 | -0.653 | 1.00 | 43.10 |
| ATOM | 5734 | OG1 | THR | 120 | 22.169 | -33.182 | -0.903 | 1.00 | 42.92 |
| ATOM | 5735 | CG2 | THR | 120 | 21.035 | -31.905 | 0.778  | 1.00 | 43.47 |
| ATOM | 5736 | H   | THR | 120 | 19.655 | -33.502 | -0.773 | 1.00 | 0.00  |
| ATOM | 5737 | HG1 | THR | 120 | 21.540 | -33.871 | -1.102 | 1.00 | 0.00  |
| ATOM | 5738 | N   | VAL | 121 | 21.204 | -30.228 | -3.296 | 1.00 | 41.98 |
| ATOM | 5739 | CA  | VAL | 121 | 21.768 | -29.795 | -4.572 | 1.00 | 40.71 |
| ATOM | 5740 | C   | VAL | 121 | 23.297 | -29.761 | -4.415 | 1.00 | 41.18 |
| ATOM | 5741 | O   | VAL | 121 | 23.814 | -29.571 | -3.308 | 1.00 | 40.92 |
| ATOM | 5742 | CB  | VAL | 121 | 21.239 | -28.381 | -4.968 | 1.00 | 37.68 |
| ATOM | 5743 | CG1 | VAL | 121 | 21.656 | -27.351 | -3.942 | 1.00 | 35.72 |
| ATOM | 5744 | CG2 | VAL | 121 | 21.730 | -27.992 | -6.343 | 1.00 | 35.33 |
| ATOM | 5745 | H   | VAL | 121 | 21.008 | -29.570 | -2.596 | 1.00 | 0.00  |
| ATOM | 5746 | N   | THR | 122 | 24.016 | -29.965 | -5.514 | 1.00 | 41.05 |
| ATOM | 5747 | CA  | THR | 122 | 25.472 | -29.957 | -5.485 | 1.00 | 40.41 |
| ATOM | 5748 | C   | THR | 122 | 26.008 | -28.524 | -5.583 | 1.00 | 39.50 |
| ATOM | 5749 | O   | THR | 122 | 25.556 | -27.741 | -6.420 | 1.00 | 39.00 |
| ATOM | 5750 | CB  | THR | 122 | 26.043 | -30.800 | -6.657 | 1.00 | 40.98 |
| ATOM | 5751 | OG1 | THR | 122 | 25.380 | -32.072 | -6.699 | 1.00 | 41.12 |
| ATOM | 5752 | CG2 | THR | 122 | 27.540 | -31.027 | -6.488 | 1.00 | 41.60 |
| ATOM | 5753 | H   | THR | 122 | 23.600 | -30.125 | -6.386 | 1.00 | 0.00  |
| ATOM | 5754 | HG1 | THR | 122 | 25.406 | -32.477 | -5.827 | 1.00 | 0.00  |
| ATOM | 5755 | N   | LEU | 123 | 26.910 | -28.155 | -4.678 | 1.00 | 39.39 |
| ATOM | 5756 | CA  | LEU | 123 | 27.504 | -26.822 | -4.714 | 1.00 | 40.23 |
| ATOM | 5757 | C   | LEU | 123 | 28.630 | -26.868 | -5.742 | 1.00 | 42.40 |
| ATOM | 5758 | O   | LEU | 123 | 29.346 | -27.865 | -5.833 | 1.00 | 44.09 |
| ATOM | 5759 | CB  | LEU | 123 | 28.052 | -26.421 | -3.341 | 1.00 | 37.96 |
| ATOM | 5760 | CG  | LEU | 123 | 27.009 | -26.086 | -2.277 | 1.00 | 35.34 |
| ATOM | 5761 | CD1 | LEU | 123 | 27.701 | -25.724 | -0.968 | 1.00 | 33.66 |
| ATOM | 5762 | CD2 | LEU | 123 | 26.133 | -24.940 | -2.768 | 1.00 | 34.28 |
| ATOM | 5763 | H   | LEU | 123 | 27.188 | -28.787 | -3.984 | 1.00 | 0.00  |
| ATOM | 5764 | N   | PRO | 124 | 28.797 | -25.797 | -6.532 | 1.00 | 43.59 |
| ATOM | 5765 | CA  | PRO | 124 | 29.845 | -25.751 | -7.556 | 1.00 | 44.65 |
| ATOM | 5766 | C   | PRO | 124 | 31.244 | -25.806 | -6.961 | 1.00 | 46.53 |
| ATOM | 5767 | O   | PRO | 124 | 31.446 | -25.467 | -5.794 | 1.00 | 46.35 |
| ATOM | 5768 | CB  | PRO | 124 | 29.611 | -24.392 | -8.227 | 1.00 | 43.56 |
| ATOM | 5769 | CG  | PRO | 124 | 28.189 | -24.090 | -7.937 | 1.00 | 43.21 |
| ATOM | 5770 | CD  | PRO | 124 | 28.051 | -24.533 | -6.511 | 1.00 | 43.13 |
| ATOM | 5771 | N   | PRO | 125 | 32.221 | -26.304 | -7.739 | 1.00 | 48.34 |
| ATOM | 5772 | CA  | PRO | 125 | 33.593 | -26.372 | -7.236 | 1.00 | 49.46 |
| ATOM | 5773 | C   | PRO | 125 | 34.145 | -24.959 | -7.385 | 1.00 | 51.62 |
| ATOM | 5774 | O   | PRO | 125 | 33.930 | -24.314 | -8.413 | 1.00 | 51.76 |
| ATOM | 5775 | CB  | PRO | 125 | 34.260 | -27.346 | -8.206 | 1.00 | 48.62 |
| ATOM | 5776 | CG  | PRO | 125 | 33.554 | -27.066 | -9.490 | 1.00 | 48.59 |

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|      |      |     |     |     |        |         |         |      |       |
|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 5777 | CD  | PRO | 125 | 32.109 | -26.934 | -9.068  | 1.00 | 48.35 |
| ATOM | 5778 | N   | ALA | 126 | 34.835 | -24.477 | -6.358  | 1.00 | 53.46 |
| ATOM | 5779 | CA  | ALA | 126 | 35.403 | -23.129 | -6.340  | 1.00 | 55.18 |
| ATOM | 5780 | C   | ALA | 126 | 35.879 | -22.583 | -7.688  | 1.00 | 56.61 |
| ATOM | 5781 | O   | ALA | 126 | 35.784 | -21.381 | -7.946  | 1.00 | 56.83 |
| ATOM | 5782 | CB  | ALA | 126 | 36.534 | -23.062 | -5.316  | 1.00 | 55.44 |
| ATOM | 5783 | H   | ALA | 126 | 34.940 | -25.053 | -5.575  | 1.00 | 0.00  |
| ATOM | 5784 | N   | SER | 127 | 36.382 | -23.472 | -8.537  | 1.00 | 58.04 |
| ATOM | 5785 | CA  | SER | 127 | 36.899 | -23.095 | -9.844  | 1.00 | 59.60 |
| ATOM | 5786 | C   | SER | 127 | 35.860 | -22.907 | -10.952 | 1.00 | 59.72 |
| ATOM | 5787 | O   | SER | 127 | 36.001 | -22.006 | -11.784 | 1.00 | 59.90 |
| ATOM | 5788 | CB  | SER | 127 | 37.948 | -24.121 | -10.294 | 1.00 | 61.16 |
| ATOM | 5789 | OG  | SER | 127 | 38.447 | -23.838 | -11.593 | 1.00 | 62.91 |
| ATOM | 5790 | H   | SER | 127 | 36.406 | -24.411 | -8.294  | 1.00 | 0.00  |
| ATOM | 5791 | HG  | SER | 127 | 39.189 | -24.409 | -11.804 | 1.00 | 0.00  |
| ATOM | 5792 | N   | GLU | 128 | 34.818 | -23.735 | -10.958 | 1.00 | 59.72 |
| ATOM | 5793 | CA  | GLU | 128 | 33.809 | -23.660 | -12.011 | 1.00 | 59.04 |
| ATOM | 5794 | C   | GLU | 128 | 33.243 | -22.269 | -12.259 | 1.00 | 56.97 |
| ATOM | 5795 | O   | GLU | 128 | 32.951 | -21.512 | -11.326 | 1.00 | 57.16 |
| ATOM | 5796 | CB  | GLU | 128 | 32.668 | -24.656 | -11.776 | 1.00 | 60.16 |
| ATOM | 5797 | CG  | GLU | 128 | 31.697 | -24.793 | -12.960 | 1.00 | 61.94 |
| ATOM | 5798 | CD  | GLU | 128 | 32.367 | -25.296 | -14.238 | 1.00 | 62.83 |
| ATOM | 5799 | OE1 | GLU | 128 | 32.175 | -26.482 | -14.587 | 1.00 | 63.13 |
| ATOM | 5800 | OE2 | GLU | 128 | 33.082 | -24.509 | -14.894 | 1.00 | 63.33 |
| ATOM | 5801 | H   | GLU | 128 | 34.671 | -24.348 | -10.221 | 1.00 | 0.00  |
| ATOM | 5802 | N   | THR | 129 | 33.118 | -21.943 | -13.538 | 1.00 | 53.80 |
| ATOM | 5803 | CA  | THR | 129 | 32.582 | -20.671 | -13.967 | 1.00 | 50.57 |
| ATOM | 5804 | C   | THR | 129 | 31.364 | -20.994 | -14.820 | 1.00 | 48.22 |
| ATOM | 5805 | O   | THR | 129 | 31.284 | -22.064 | -15.428 | 1.00 | 48.65 |
| ATOM | 5806 | CB  | THR | 129 | 33.618 | -19.875 | -14.787 | 1.00 | 50.61 |
| ATOM | 5807 | OG1 | THR | 129 | 33.061 | -18.605 | -15.153 | 1.00 | 50.73 |
| ATOM | 5808 | CG2 | THR | 129 | 34.032 | -20.640 | -16.047 | 1.00 | 50.35 |
| ATOM | 5809 | H   | THR | 129 | 33.330 | -22.630 | -14.214 | 1.00 | 0.00  |
| ATOM | 5810 | HG1 | THR | 129 | 33.746 | -17.950 | -14.971 | 1.00 | 0.00  |
| ATOM | 5811 | N   | PHE | 130 | 30.397 | -20.088 | -14.843 | 1.00 | 44.03 |
| ATOM | 5812 | CA  | PHE | 130 | 29.196 | -20.311 | -15.627 | 1.00 | 40.01 |
| ATOM | 5813 | C   | PHE | 130 | 29.147 | -19.285 | -16.745 | 1.00 | 40.47 |
| ATOM | 5814 | O   | PHE | 130 | 28.598 | -18.192 | -16.587 | 1.00 | 40.48 |
| ATOM | 5815 | CB  | PHE | 130 | 27.968 | -20.245 | -14.729 | 1.00 | 34.57 |
| ATOM | 5816 | CG  | PHE | 130 | 28.014 | -21.229 | -13.612 | 1.00 | 29.00 |
| ATOM | 5817 | CD1 | PHE | 130 | 28.561 | -20.877 | -12.388 | 1.00 | 27.62 |
| ATOM | 5818 | CD2 | PHE | 130 | 27.577 | -22.527 | -13.801 | 1.00 | 26.57 |
| ATOM | 5819 | CE1 | PHE | 130 | 28.682 | -21.810 | -11.366 | 1.00 | 26.04 |
| ATOM | 5820 | CE2 | PHE | 130 | 27.694 | -23.465 | -12.787 | 1.00 | 26.00 |
| ATOM | 5821 | CZ  | PHE | 130 | 28.249 | -23.106 | -11.566 | 1.00 | 25.15 |
| ATOM | 5822 | H   | PHE | 130 | 30.518 | -19.245 | -14.371 | 1.00 | 0.00  |
| ATOM | 5823 | N   | PRO | 131 | 29.785 | -19.612 | -17.878 | 1.00 | 40.90 |
| ATOM | 5824 | CA  | PRO | 131 | 29.866 | -18.772 | -19.070 | 1.00 | 40.56 |
| ATOM | 5825 | C   | PRO | 131 | 28.495 | -18.495 | -19.624 | 1.00 | 40.93 |
| ATOM | 5826 | O   | PRO | 131 | 27.550 | -19.250 | -19.389 | 1.00 | 40.50 |
| ATOM | 5827 | CB  | PRO | 131 | 30.660 | -19.640 | -20.044 | 1.00 | 41.58 |
| ATOM | 5828 | CG  | PRO | 131 | 31.489 | -20.487 | -19.153 | 1.00 | 42.76 |
| ATOM | 5829 | CD  | PRO | 131 | 30.487 | -20.882 | -18.110 | 1.00 | 41.43 |
| ATOM | 5830 | N   | PRO | 132 | 28.362 | -17.393 | -20.366 | 1.00 | 42.09 |
| ATOM | 5831 | CA  | PRO | 132 | 27.072 | -17.041 | -20.951 | 1.00 | 43.35 |
| ATOM | 5832 | C   | PRO | 132 | 26.573 | -18.184 | -21.827 | 1.00 | 44.96 |
| ATOM | 5833 | O   | PRO | 132 | 27.369 | -18.963 | -22.357 | 1.00 | 45.53 |
| ATOM | 5834 | CB  | PRO | 132 | 27.412 | -15.809 | -21.779 | 1.00 | 42.68 |
| ATOM | 5835 | CG  | PRO | 132 | 28.507 | -15.165 | -20.976 | 1.00 | 42.74 |
| ATOM | 5836 | CD  | PRO | 132 | 29.367 | -16.349 | -20.628 | 1.00 | 42.36 |
| ATOM | 5837 | N   | GLY | 133 | 25.255 | -18.303 | -21.941 | 1.00 | 46.46 |
| ATOM | 5838 | CA  | GLY | 133 | 24.676 | -19.352 | -22.760 | 1.00 | 47.33 |
| ATOM | 5839 | C   | GLY | 133 | 24.737 | -20.731 | -22.135 | 1.00 | 47.78 |

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|      |      |     |     |     |        |         |         |      |       |
|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 5840 | O   | GLY | 133 | 24.897 | -21.729 | -22.837 | 1.00 | 47.69 |
| ATOM | 5841 | H   | GLY | 133 | 24.704 | -17.646 | -21.466 | 1.00 | 0.00  |
| ATOM | 5842 | N   | MET | 134 | 24.608 | -20.791 | -20.816 | 1.00 | 48.51 |
| ATOM | 5843 | CA  | MET | 134 | 24.625 | -22.067 | -20.110 | 1.00 | 48.72 |
| ATOM | 5844 | C   | MET | 134 | 23.191 | -22.373 | -19.640 | 1.00 | 48.89 |
| ATOM | 5845 | O   | MET | 134 | 22.452 | -21.461 | -19.236 | 1.00 | 48.99 |
| ATOM | 5846 | CB  | MET | 134 | 25.591 | -22.002 | -18.921 | 1.00 | 47.99 |
| ATOM | 5847 | CG  | MET | 134 | 25.892 | -23.340 | -18.279 | 1.00 | 47.43 |
| ATOM | 5848 | SD  | MET | 134 | 27.053 | -23.199 | -16.914 | 1.00 | 49.72 |
| ATOM | 5849 | CE  | MET | 134 | 28.548 | -23.664 | -17.723 | 1.00 | 49.32 |
| ATOM | 5850 | H   | MET | 134 | 24.498 | -19.978 | -20.291 | 1.00 | 0.00  |
| ATOM | 5851 | N   | PRO | 135 | 22.761 | -23.647 | -19.749 | 1.00 | 48.26 |
| ATOM | 5852 | CA  | PRO | 135 | 21.417 | -24.074 | -19.339 | 1.00 | 45.81 |
| ATOM | 5853 | C   | PRO | 135 | 21.195 | -23.868 | -17.846 | 1.00 | 42.66 |
| ATOM | 5854 | O   | PRO | 135 | 21.483 | -24.751 | -17.030 | 1.00 | 42.66 |
| ATOM | 5855 | CB  | PRO | 135 | 21.403 | -25.560 | -19.712 | 1.00 | 46.98 |
| ATOM | 5856 | CG  | PRO | 135 | 22.848 | -25.962 | -19.576 | 1.00 | 47.30 |
| ATOM | 5857 | CD  | PRO | 135 | 23.539 | -24.799 | -20.245 | 1.00 | 48.97 |
| ATOM | 5858 | N   | CYS | 136 | 20.720 | -22.684 | -17.492 | 1.00 | 38.45 |
| ATOM | 5859 | CA  | CYS | 136 | 20.476 | -22.372 | -16.104 | 1.00 | 35.63 |
| ATOM | 5860 | C   | CYS | 136 | 19.000 | -22.143 | -15.849 | 1.00 | 33.86 |
| ATOM | 5861 | O   | CYS | 136 | 18.270 | -21.663 | -16.716 | 1.00 | 32.99 |
| ATOM | 5862 | CB  | CYS | 136 | 21.314 | -21.173 | -15.696 | 1.00 | 34.89 |
| ATOM | 5863 | SG  | CYS | 136 | 23.091 | -21.482 | -15.932 | 1.00 | 35.41 |
| ATOM | 5864 | H   | CYS | 136 | 20.545 | -21.978 | -18.151 | 1.00 | 0.00  |
| ATOM | 5865 | N   | TRP | 137 | 18.556 | -22.537 | -14.665 | 1.00 | 31.87 |
| ATOM | 5866 | CA  | TRP | 137 | 17.166 | -22.397 | -14.295 | 1.00 | 31.35 |
| ATOM | 5867 | C   | TRP | 137 | 17.006 | -21.877 | -12.887 | 1.00 | 31.64 |
| ATOM | 5868 | O   | TRP | 137 | 17.790 | -22.218 | -11.999 | 1.00 | 32.59 |
| ATOM | 5869 | CB  | TRP | 137 | 16.478 | -23.752 | -14.353 | 1.00 | 32.22 |
| ATOM | 5870 | CG  | TRP | 137 | 16.346 | -24.327 | -15.700 | 1.00 | 32.31 |
| ATOM | 5871 | CD1 | TRP | 137 | 17.334 | -24.876 | -16.457 | 1.00 | 32.28 |
| ATOM | 5872 | CD2 | TRP | 137 | 15.132 | -24.491 | -16.433 | 1.00 | 32.79 |
| ATOM | 5873 | NE1 | TRP | 137 | 16.809 | -25.385 | -17.617 | 1.00 | 33.38 |
| ATOM | 5874 | CE2 | TRP | 137 | 15.456 | -25.163 | -17.629 | 1.00 | 33.14 |
| ATOM | 5875 | CE3 | TRP | 137 | 13.796 | -24.143 | -16.191 | 1.00 | 33.80 |
| ATOM | 5876 | CZ2 | TRP | 137 | 14.492 | -25.497 | -18.587 | 1.00 | 34.85 |
| ATOM | 5877 | CZ3 | TRP | 137 | 12.834 | -24.475 | -17.145 | 1.00 | 35.45 |
| ATOM | 5878 | CH2 | TRP | 137 | 13.189 | -25.146 | -18.330 | 1.00 | 35.55 |
| ATOM | 5879 | H   | TRP | 137 | 19.178 | -22.948 | -14.032 | 1.00 | 0.00  |
| ATOM | 5880 | HE1 | TRP | 137 | 17.333 | -25.845 | -18.304 | 1.00 | 0.00  |
| ATOM | 5881 | N   | VAL | 138 | 15.971 | -21.064 | -12.693 | 1.00 | 31.34 |
| ATOM | 5882 | CA  | VAL | 138 | 15.631 | -20.511 | -11.384 | 1.00 | 31.07 |
| ATOM | 5883 | C   | VAL | 138 | 14.219 | -21.012 | -11.098 | 1.00 | 30.96 |
| ATOM | 5884 | O   | VAL | 138 | 13.423 | -21.202 | -12.030 | 1.00 | 31.00 |
| ATOM | 5885 | CB  | VAL | 138 | 15.663 | -18.958 | -11.347 | 1.00 | 30.99 |
| ATOM | 5886 | CG1 | VAL | 138 | 17.088 | -18.458 | -11.387 | 1.00 | 32.21 |
| ATOM | 5887 | CG2 | VAL | 138 | 14.895 | -18.379 | -12.505 | 1.00 | 32.19 |
| ATOM | 5888 | H   | VAL | 138 | 15.405 | -20.881 | -13.475 | 1.00 | 0.00  |
| ATOM | 5889 | N   | THR | 139 | 13.927 | -21.271 | -9.827  | 1.00 | 29.92 |
| ATOM | 5890 | CA  | THR | 139 | 12.620 | -21.779 | -9.422  | 1.00 | 29.41 |
| ATOM | 5891 | C   | THR | 139 | 12.161 | -21.166 | -8.097  | 1.00 | 29.36 |
| ATOM | 5892 | O   | THR | 139 | 12.985 | -20.914 | -7.207  | 1.00 | 30.92 |
| ATOM | 5893 | CB  | THR | 139 | 12.646 | -23.326 | -9.287  | 1.00 | 29.70 |
| ATOM | 5894 | OG1 | THR | 139 | 13.722 | -23.724 | -8.421  | 1.00 | 30.69 |
| ATOM | 5895 | CG2 | THR | 139 | 12.853 | -23.975 | -10.640 | 1.00 | 28.79 |
| ATOM | 5896 | H   | THR | 139 | 14.619 | -21.111 | -9.150  | 1.00 | 0.00  |
| ATOM | 5897 | HG1 | THR | 139 | 13.914 | -22.990 | -7.822  | 1.00 | 0.00  |
| ATOM | 5898 | N   | GLY | 140 | 10.856 | -20.950 | -7.956  | 1.00 | 26.95 |
| ATOM | 5899 | CA  | GLY | 140 | 10.336 | -20.372 | -6.729  | 1.00 | 25.57 |
| ATOM | 5900 | C   | GLY | 140 | 8.842  | -20.154 | -6.781  | 1.00 | 24.27 |
| ATOM | 5901 | O   | GLY | 140 | 8.189  | -20.574 | -7.732  | 1.00 | 25.57 |
| ATOM | 5902 | H   | GLY | 140 | 10.227 | -21.181 | -8.680  | 1.00 | 0.00  |

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|      |      |      |     |     |       |         |         |      |       |
|------|------|------|-----|-----|-------|---------|---------|------|-------|
| ATOM | 5903 | N    | TRP | 141 | 8.295 | -19.534 | -5.740  | 1.00 | 22.20 |
| ATOM | 5904 | CA   | TRP | 141 | 6.865 | -19.248 | -5.665  | 1.00 | 20.99 |
| ATOM | 5905 | C    | TRP | 141 | 6.623 | -17.737 | -5.642  | 1.00 | 21.65 |
| ATOM | 5906 | O    | TRP | 141 | 5.714 | -17.256 | -4.948  | 1.00 | 23.36 |
| ATOM | 5907 | CB   | TRP | 141 | 6.282 | -19.821 | -4.380  | 1.00 | 19.03 |
| ATOM | 5908 | CG   | TRP | 141 | 6.102 | -21.283 | -4.345  | 1.00 | 18.34 |
| ATOM | 5909 | CD1  | TRP | 141 | 5.003 | -21.980 | -4.759  | 1.00 | 18.69 |
| ATOM | 5910 | CD2  | TRP | 141 | 6.975 | -22.235 | -3.735  | 1.00 | 17.69 |
| ATOM | 5911 | NE1  | TRP | 141 | 5.130 | -23.302 | -4.425  | 1.00 | 18.32 |
| ATOM | 5912 | CE2  | TRP | 141 | 6.333 | -23.487 | -3.794  | 1.00 | 18.19 |
| ATOM | 5913 | CE3  | TRP | 141 | 8.233 | -22.149 | -3.128  | 1.00 | 16.74 |
| ATOM | 5914 | CZ2  | TRP | 141 | 6.908 | -24.644 | -3.267  | 1.00 | 17.70 |
| ATOM | 5915 | CZ3  | TRP | 141 | 8.801 | -23.298 | -2.604  | 1.00 | 15.78 |
| ATOM | 5916 | CH2  | TRP | 141 | 8.138 | -24.528 | -2.676  | 1.00 | 16.93 |
| ATOM | 5917 | H    | TRP | 141 | 8.899 | -19.228 | -5.036  | 1.00 | 0.00  |
| ATOM | 5918 | HE1  | TRP | 141 | 4.448 | -23.975 | -4.652  | 1.00 | 0.00  |
| ATOM | 5919 | N    | GLY | 142 | 7.441 | -16.986 | -6.369  | 1.00 | 19.98 |
| ATOM | 5920 | CA   | GLY | 142 | 7.299 | -15.544 | -6.368  | 1.00 | 18.55 |
| ATOM | 5921 | C    | GLY | 142 | 6.288 | -14.924 | -7.306  | 1.00 | 18.04 |
| ATOM | 5922 | O    | GLY | 142 | 5.475 | -15.607 | -7.930  | 1.00 | 16.94 |
| ATOM | 5923 | H    | GLY | 142 | 8.167 | -17.369 | -6.913  | 1.00 | 0.00  |
| ATOM | 5924 | N    | ASP | 143 | 6.314 | -13.598 | -7.347  | 1.00 | 19.03 |
| ATOM | 5925 | CA   | ASP | 143 | 5.433 | -12.835 | -8.208  | 1.00 | 21.24 |
| ATOM | 5926 | C    | ASP | 143 | 5.745 | -13.248 | -9.624  | 1.00 | 22.79 |
| ATOM | 5927 | O    | ASP | 143 | 6.909 | -13.422 | -9.990  | 1.00 | 23.16 |
| ATOM | 5928 | CB   | ASP | 143 | 5.686 | -11.334 | -8.057  | 1.00 | 21.71 |
| ATOM | 5929 | CG   | ASP | 143 | 5.148 | -10.769 | -6.751  | 1.00 | 23.33 |
| ATOM | 5930 | OD1  | ASP | 143 | 4.618 | -11.540 | -5.913  | 1.00 | 23.76 |
| ATOM | 5931 | OD2  | ASP | 143 | 5.258 | -9.535  | -6.565  | 1.00 | 23.38 |
| ATOM | 5932 | H    | ASP | 143 | 6.930 | -13.138 | -6.757  | 1.00 | 0.00  |
| ATOM | 5933 | N    | VAL | 144 | 4.699 | -13.391 | -10.421 | 1.00 | 24.07 |
| ATOM | 5934 | CA   | VAL | 144 | 4.854 | -13.782 | -11.807 | 1.00 | 25.12 |
| ATOM | 5935 | C    | VAL | 144 | 4.991 | -12.545 | -12.688 | 1.00 | 27.21 |
| ATOM | 5936 | O    | VAL | 144 | 5.038 | -12.644 | -13.915 | 1.00 | 27.06 |
| ATOM | 5937 | CB   | VAL | 144 | 3.685 | -14.640 | -12.247 | 1.00 | 23.86 |
| ATOM | 5938 | CG1  | VAL | 144 | 3.616 | -15.889 | -11.373 | 1.00 | 23.15 |
| ATOM | 5939 | CG2  | VAL | 144 | 2.401 | -13.844 | -12.146 | 1.00 | 24.15 |
| ATOM | 5940 | H    | VAL | 144 | 3.838 | -13.140 | -10.028 | 1.00 | 0.00  |
| ATOM | 5941 | N    | ASP | 145 | 5.038 | -11.389 | -12.032 | 1.00 | 30.21 |
| ATOM | 5942 | CA   | ASP | 145 | 5.208 | -10.084 | -12.662 | 1.00 | 32.95 |
| ATOM | 5943 | C    | ASP | 145 | 5.186 | -9.056  | -11.532 | 1.00 | 33.80 |
| ATOM | 5944 | O    | ASP | 145 | 4.771 | -9.360  | -10.407 | 1.00 | 34.03 |
| ATOM | 5945 | CB   | ASP | 145 | 4.089 | -9.794  | -13.667 | 1.00 | 35.68 |
| ATOM | 5946 | CG   | ASP | 145 | 4.501 | -8.777  | -14.733 | 1.00 | 40.39 |
| ATOM | 5947 | OD1  | ASP | 145 | 5.163 | -7.773  | -14.397 | 1.00 | 41.50 |
| ATOM | 5948 | OD2  | ASP | 145 | 4.176 | -8.983  | -15.923 | 1.00 | 43.13 |
| ATOM | 5949 | H    | ASP | 145 | 4.923 | -11.365 | -11.060 | 1.00 | 0.00  |
| ATOM | 5950 | N    | ASN | 146 | 5.692 | -7.863  | -11.800 | 1.00 | 35.25 |
| ATOM | 5951 | CA   | ASN | 146 | 5.707 | -6.808  | -10.800 | 1.00 | 37.85 |
| ATOM | 5952 | C    | ASN | 146 | 4.263 | -6.542  | -10.371 | 1.00 | 39.69 |
| ATOM | 5953 | O    | ASN | 146 | 3.368 | -6.411  | -11.211 | 1.00 | 38.91 |
| ATOM | 5954 | CB   | ASN | 146 | 6.327 | -5.527  | -11.377 | 1.00 | 38.72 |
| ATOM | 5955 | CG   | ASN | 146 | 7.818 | -5.665  | -11.688 | 1.00 | 39.84 |
| ATOM | 5956 | OD1  | ASN | 146 | 8.274 | -6.678  | -12.215 | 1.00 | 39.84 |
| ATOM | 5957 | ND2  | ASN | 146 | 8.582 | -4.630  | -11.363 | 1.00 | 40.72 |
| ATOM | 5958 | H    | ASN | 146 | 6.039 | -7.698  | -12.700 | 1.00 | 0.00  |
| ATOM | 5959 | HD21 | ASN | 146 | 8.150 | -3.870  | -10.922 | 1.00 | 0.00  |
| ATOM | 5960 | HD22 | ASN | 146 | 9.531 | -4.627  | -11.582 | 1.00 | 0.00  |
| ATOM | 5961 | N    | ASP | 147 | 4.041 | -6.510  | -9.061  | 1.00 | 42.92 |
| ATOM | 5962 | CA   | ASP | 147 | 2.720 | -6.271  | -8.481  | 1.00 | 45.50 |
| ATOM | 5963 | C    | ASP | 147 | 1.678 | -7.310  | -8.888  | 1.00 | 45.08 |
| ATOM | 5964 | O    | ASP | 147 | 0.491 | -7.005  | -9.009  | 1.00 | 45.63 |
| ATOM | 5965 | CB   | ASP | 147 | 2.224 | -4.854  | -8.801  | 1.00 | 49.17 |

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|      |      |      |     |      |        |         |         |      |       |
|------|------|------|-----|------|--------|---------|---------|------|-------|
| ATOM | 5966 | CG   | ASP | 147  | 3.135  | -3.776  | -8.242  | 1.00 | 51.28 |
| ATOM | 5967 | OD1  | ASP | 147  | 3.564  | -3.892  | -7.069  | 1.00 | 51.76 |
| ATOM | 5968 | OD2  | ASP | 147  | 3.432  | -2.814  | -8.983  | 1.00 | 52.33 |
| ATOM | 5969 | H    | ASP | 147  | 4.782  | -6.628  | -8.446  | 1.00 | 0.00  |
| ATOM | 5970 | N    | GLU | 149  | 2.132  | -8.549  | -9.050  | 1.00 | 44.34 |
| ATOM | 5971 | CA   | GLU | 149  | 1.274  | -9.668  | -9.422  | 1.00 | 44.10 |
| ATOM | 5972 | C    | GLU | 149  | 1.644  | -10.870 | -8.552  | 1.00 | 44.12 |
| ATOM | 5973 | O    | GLU | 149  | 2.603  | -11.588 | -8.862  | 1.00 | 45.54 |
| ATOM | 5974 | CB   | GLU | 149  | 1.485  | -10.021 | -10.895 | 1.00 | 44.59 |
| ATOM | 5975 | CG   | GLU | 149  | 0.598  | -9.275  | -11.856 | 1.00 | 45.44 |
| ATOM | 5976 | CD   | GLU | 149  | -0.686 | -10.014 | -12.112 | 1.00 | 46.55 |
| ATOM | 5977 | OE1  | GLU | 149  | -1.673 | -9.754  | -11.396 | 1.00 | 47.85 |
| ATOM | 5978 | OE2  | GLU | 149  | -0.705 | -10.864 | -13.028 | 1.00 | 47.49 |
| ATOM | 5979 | H    | GLU | 149  | 3.092  | -8.734  | -8.946  | 1.00 | 0.00  |
| ATOM | 5980 | N    | ARG | 150  | 0.898  | -11.083 | -7.469  | 1.00 | 42.34 |
| ATOM | 5981 | CA   | ARG | 150  | 1.173  | -12.192 | -6.562  | 1.00 | 40.58 |
| ATOM | 5982 | C    | ARG | 150  | 0.909  | -13.510 | -7.271  | 1.00 | 36.71 |
| ATOM | 5983 | O    | ARG | 150  | 0.113  | -13.567 | -8.202  | 1.00 | 35.51 |
| ATOM | 5984 | CB   | ARG | 150  | 0.299  | -12.076 | -5.298  | 1.00 | 44.36 |
| ATOM | 5985 | CG   | ARG | 150  | 0.983  | -12.449 | -3.958  | 1.00 | 49.52 |
| ATOM | 5986 | CD   | ARG | 150  | 0.705  | -13.891 | -3.461  | 1.00 | 52.52 |
| ATOM | 5987 | NE   | ARG | 150  | 1.800  | -14.823 | -3.749  | 1.00 | 56.25 |
| ATOM | 5988 | CZ   | ARG | 150  | 2.116  | -15.884 | -3.004  | 1.00 | 57.81 |
| ATOM | 5989 | NH1  | ARG | 150  | 1.418  | -16.165 | -1.904  | 1.00 | 58.65 |
| ATOM | 5990 | NH2  | ARG | 150  | 3.149  | -16.654 | -3.345  | 1.00 | 58.09 |
| ATOM | 5991 | H    | ARG | 150  | 0.136  | -10.505 | -7.318  | 1.00 | 0.00  |
| ATOM | 5992 | HE   | ARG | 150  | 2.358  | -14.637 | -4.544  | 1.00 | 0.00  |
| ATOM | 5993 | HH11 | ARG | 150  | 0.638  | -15.589 | -1.639  | 1.00 | 0.00  |
| ATOM | 5994 | HH12 | ARG | 150  | 1.629  | -16.941 | -1.289  | 1.00 | 0.00  |
| ATOM | 5995 | HH21 | ARG | 150  | 3.733  | -16.457 | -4.142  | 1.00 | 0.00  |
| ATOM | 5996 | HH22 | ARG | 150  | 3.419  | -17.458 | -2.818  | 1.00 | 0.00  |
| ATOM | 5997 | N    | LEU | 151  | 1.612  | -14.558 | -6.864  | 1.00 | 33.64 |
| ATOM | 5998 | CA   | LEU | 151  | 1.437  | -15.887 | -7.439  | 1.00 | 31.59 |
| ATOM | 5999 | C    | LEU | 151  | 0.033  | -16.344 | -7.041  | 1.00 | 31.86 |
| ATOM | 6000 | O    | LEU | 151  | -0.236 | -16.555 | -5.857  | 1.00 | 33.16 |
| ATOM | 6001 | CB   | LEU | 151  | 2.468  | -16.854 | -6.853  | 1.00 | 28.75 |
| ATOM | 6002 | CG   | LEU | 151  | 2.340  | -18.312 | -7.296  | 1.00 | 27.73 |
| ATOM | 6003 | CD1  | LEU | 151  | 2.701  | -18.464 | -8.770  | 1.00 | 26.76 |
| ATOM | 6004 | CD2  | LEU | 151  | 3.235  | -19.164 | -6.431  | 1.00 | 26.77 |
| ATOM | 6005 | H    | LEU | 151  | 2.315  | -14.446 | -6.184  | 1.00 | 0.00  |
| ATOM | 6006 | N    | PRO | 152  | -0.866 | -16.531 | -8.023  | 1.00 | 31.21 |
| ATOM | 6007 | CA   | PRO | 152  | -2.248 | -16.957 | -7.774  | 1.00 | 30.53 |
| ATOM | 6008 | C    | PRO | 152  | -2.375 | -18.369 | -7.228  | 1.00 | 30.09 |
| ATOM | 6009 | O    | PRO | 152  | -1.578 | -19.254 | -7.555  | 1.00 | 30.99 |
| ATOM | 6010 | CB   | PRO | 152  | -2.890 | -16.883 | -9.162  | 1.00 | 30.77 |
| ATOM | 6011 | CG   | PRO | 152  | -1.984 | -15.982 | -9.942  | 1.00 | 31.82 |
| ATOM | 6012 | CD   | PRO | 152  | -0.632 | -16.410 | -9.464  | 1.00 | 31.49 |
| ATOM | 6013 | N    | PRO | 152A | -3.389 | -18.600 | -6.387  | 1.00 | 28.14 |
| ATOM | 6014 | CA   | PRO | 152A | -3.665 | -19.901 | -5.773  | 1.00 | 27.11 |
| ATOM | 6015 | C    | PRO | 152A | -3.922 | -20.895 | -6.891  | 1.00 | 25.31 |
| ATOM | 6016 | O    | PRO | 152A | -4.539 | -20.534 | -7.892  | 1.00 | 24.42 |
| ATOM | 6017 | CB   | PRO | 152A | -4.944 | -19.627 | -4.993  | 1.00 | 27.02 |
| ATOM | 6018 | CG   | PRO | 152A | -4.795 | -18.202 | -4.600  | 1.00 | 27.30 |
| ATOM | 6019 | CD   | PRO | 152A | -4.319 | -17.580 | -5.883  | 1.00 | 28.07 |
| ATOM | 6020 | N    | PRO | 152B | -3.446 | -22.149 | -6.756  | 1.00 | 24.63 |
| ATOM | 6021 | CA   | PRO | 152B | -2.955 | -22.907 | -5.600  | 1.00 | 24.72 |
| ATOM | 6022 | C    | PRO | 152B | -1.463 | -22.757 | -5.251  | 1.00 | 25.47 |
| ATOM | 6023 | O    | PRO | 152B | -0.897 | -23.628 | -4.580  | 1.00 | 26.39 |
| ATOM | 6024 | CB   | PRO | 152B | -3.245 | -24.338 | -6.021  | 1.00 | 24.31 |
| ATOM | 6025 | CG   | PRO | 152B | -2.897 | -24.313 | -7.448  | 1.00 | 23.77 |
| ATOM | 6026 | CD   | PRO | 152B | -3.581 | -23.048 | -7.919  | 1.00 | 25.10 |
| ATOM | 6027 | N    | PHE | 153  | -0.821 | -21.697 | -5.745  | 1.00 | 24.43 |
| ATOM | 6028 | CA   | PHE | 153  | 0.596  | -21.418 | -5.486  | 1.00 | 22.49 |

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|      |      |      |     |     |        |         |         |      |       |
|------|------|------|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6029 | C    | PHE | 153 | 1.542  | -22.546 | -5.917  | 1.00 | 22.52 |
| ATOM | 6030 | O    | PHE | 153 | 2.274  | -23.118 | -5.098  | 1.00 | 23.36 |
| ATOM | 6031 | CB   | PHE | 153 | 0.815  | -21.105 | -4.009  | 1.00 | 19.70 |
| ATOM | 6032 | CG   | PHE | 153 | -0.229 | -20.218 | -3.425  | 1.00 | 19.12 |
| ATOM | 6033 | CD1  | PHE | 153 | -1.208 | -20.739 | -2.592  | 1.00 | 18.41 |
| ATOM | 6034 | CD2  | PHE | 153 | -0.230 | -18.857 | -3.691  | 1.00 | 19.19 |
| ATOM | 6035 | CE1  | PHE | 153 | -2.169 | -19.923 | -2.031  | 1.00 | 18.36 |
| ATOM | 6036 | CE2  | PHE | 153 | -1.189 | -18.027 | -3.133  | 1.00 | 18.48 |
| ATOM | 6037 | CZ   | PHE | 153 | -2.159 | -18.559 | -2.303  | 1.00 | 18.33 |
| ATOM | 6038 | H    | PHE | 153 | -1.258 | -21.053 | -6.341  | 1.00 | 0.00  |
| ATOM | 6039 | N    | PRO | 154 | 1.539  | -22.877 | -7.213  | 1.00 | 21.19 |
| ATOM | 6040 | CA   | PRO | 154 | 2.399  | -23.938 | -7.737  | 1.00 | 20.90 |
| ATOM | 6041 | C    | PRO | 154 | 3.838  | -23.468 | -7.807  | 1.00 | 21.87 |
| ATOM | 6042 | O    | PRO | 154 | 4.105  | -22.268 | -7.820  | 1.00 | 23.46 |
| ATOM | 6043 | CB   | PRO | 154 | 1.843  | -24.145 | -9.134  | 1.00 | 20.95 |
| ATOM | 6044 | CG   | PRO | 154 | 1.490  | -22.747 | -9.541  | 1.00 | 21.55 |
| ATOM | 6045 | CD   | PRO | 154 | 0.808  | -22.206 | -8.304  | 1.00 | 20.85 |
| ATOM | 6046 | N    | LEU | 155 | 4.767  | -24.409 | -7.845  | 1.00 | 22.18 |
| ATOM | 6047 | CA   | LEU | 155 | 6.182  | -24.060 | -7.947  | 1.00 | 21.41 |
| ATOM | 6048 | C    | LEU | 155 | 6.453  | -23.788 | -9.418  | 1.00 | 21.00 |
| ATOM | 6049 | O    | LEU | 155 | 6.141  | -24.614 | -10.272 | 1.00 | 21.98 |
| ATOM | 6050 | CB   | LEU | 155 | 7.054  | -25.227 | -7.482  | 1.00 | 19.20 |
| ATOM | 6051 | CG   | LEU | 155 | 8.568  | -25.064 | -7.538  | 1.00 | 16.60 |
| ATOM | 6052 | CD1  | LEU | 155 | 9.046  | -24.292 | -6.331  | 1.00 | 17.48 |
| ATOM | 6053 | CD2  | LEU | 155 | 9.206  | -26.430 | -7.551  | 1.00 | 17.11 |
| ATOM | 6054 | H    | LEU | 155 | 4.496  | -25.345 | -7.794  | 1.00 | 0.00  |
| ATOM | 6055 | N    | LYS | 156 | 6.995  | -22.624 | -9.730  | 1.00 | 20.69 |
| ATOM | 6056 | CA   | LYS | 156 | 7.289  | -22.314 | -11.115 | 1.00 | 20.73 |
| ATOM | 6057 | C    | LYS | 156 | 8.772  | -22.479 | -11.371 | 1.00 | 20.75 |
| ATOM | 6058 | O    | LYS | 156 | 9.570  | -22.526 | -10.437 | 1.00 | 21.16 |
| ATOM | 6059 | CB   | LYS | 156 | 6.851  | -20.896 | -11.460 | 1.00 | 21.65 |
| ATOM | 6060 | CG   | LYS | 156 | 5.351  | -20.679 | -11.375 | 1.00 | 23.13 |
| ATOM | 6061 | CD   | LYS | 156 | 4.960  | -19.436 | -12.144 | 1.00 | 24.97 |
| ATOM | 6062 | CE   | LYS | 156 | 5.312  | -19.587 | -13.618 | 1.00 | 25.65 |
| ATOM | 6063 | NZ   | LYS | 156 | 5.198  | -18.307 | -14.370 | 1.00 | 27.51 |
| ATOM | 6064 | H    | LYS | 156 | 7.236  | -21.974 | -9.036  | 1.00 | 0.00  |
| ATOM | 6065 | HZ1  | LYS | 156 | 5.837  | -17.594 | -13.939 | 1.00 | 0.00  |
| ATOM | 6066 | HZ2  | LYS | 156 | 4.221  | -17.961 | -14.330 | 1.00 | 0.00  |
| ATOM | 6067 | HZ3  | LYS | 156 | 5.463  | -18.515 | -15.364 | 1.00 | 0.00  |
| ATOM | 6068 | N    | GLN | 157 | 9.134  | -22.561 | -12.640 | 1.00 | 21.24 |
| ATOM | 6069 | CA   | GLN | 157 | 10.519 | -22.717 | -13.044 | 1.00 | 22.24 |
| ATOM | 6070 | C    | GLN | 157 | 10.708 | -21.973 | -14.354 | 1.00 | 24.17 |
| ATOM | 6071 | O    | GLN | 157 | 9.763  | -21.840 | -15.133 | 1.00 | 24.32 |
| ATOM | 6072 | CB   | GLN | 157 | 10.818 | -24.191 | -13.277 | 1.00 | 21.80 |
| ATOM | 6073 | CG   | GLN | 157 | 9.846  | -24.834 | -14.247 | 1.00 | 22.41 |
| ATOM | 6074 | CD   | GLN | 157 | 10.306 | -26.182 | -14.742 | 1.00 | 23.03 |
| ATOM | 6075 | OE1  | GLN | 157 | 11.101 | -26.862 | -14.098 | 1.00 | 22.47 |
| ATOM | 6076 | NE2  | GLN | 157 | 9.805  | -26.578 | -15.898 | 1.00 | 24.40 |
| ATOM | 6077 | H    | GLN | 157 | 8.438  | -22.525 | -13.322 | 1.00 | 0.00  |
| ATOM | 6078 | HE21 | GLN | 157 | 9.159  | -25.994 | -16.343 | 1.00 | 0.00  |
| ATOM | 6079 | HE22 | GLN | 157 | 10.089 | -27.439 | -16.258 | 1.00 | 0.00  |
| ATOM | 6080 | N    | VAL | 158 | 11.914 | -21.483 | -14.600 | 1.00 | 25.41 |
| ATOM | 6081 | CA   | VAL | 158 | 12.192 | -20.794 | -15.848 | 1.00 | 26.28 |
| ATOM | 6082 | C    | VAL | 158 | 13.671 | -20.886 | -16.201 | 1.00 | 27.79 |
| ATOM | 6083 | O    | VAL | 158 | 14.521 | -20.919 | -15.310 | 1.00 | 27.83 |
| ATOM | 6084 | CB   | VAL | 158 | 11.734 | -19.331 | -15.804 | 1.00 | 26.15 |
| ATOM | 6085 | CG1  | VAL | 158 | 12.481 | -18.567 | -14.743 | 1.00 | 27.07 |
| ATOM | 6086 | CG2  | VAL | 158 | 11.910 | -18.693 | -17.163 | 1.00 | 26.67 |
| ATOM | 6087 | H    | VAL | 158 | 12.603 | -21.547 | -13.901 | 1.00 | 0.00  |
| ATOM | 6088 | N    | LYS | 159 | 13.956 | -21.018 | -17.499 | 1.00 | 29.34 |
| ATOM | 6089 | CA   | LYS | 159 | 15.324 | -21.122 | -18.003 | 1.00 | 29.35 |
| ATOM | 6090 | C    | LYS | 159 | 15.870 | -19.733 | -18.241 | 1.00 | 29.03 |
| ATOM | 6091 | O    | LYS | 159 | 15.325 | -18.968 | -19.042 | 1.00 | 29.33 |

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|      |      |      |     |     |        |         |         |      |       |
|------|------|------|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6092 | CB   | LYS | 159 | 15.380 | -21.920 | -19.312 | 1.00 | 30.80 |
| ATOM | 6093 | CG   | LYS | 159 | 16.769 | -21.929 | -19.963 | 1.00 | 33.80 |
| ATOM | 6094 | CD   | LYS | 159 | 16.998 | -23.100 | -20.938 | 1.00 | 35.63 |
| ATOM | 6095 | CE   | LYS | 159 | 16.409 | -22.874 | -22.336 | 1.00 | 37.43 |
| ATOM | 6096 | NZ   | LYS | 159 | 14.922 | -23.033 | -22.420 | 1.00 | 38.90 |
| ATOM | 6097 | H    | LYS | 159 | 13.213 | -21.008 | -18.129 | 1.00 | 0.00  |
| ATOM | 6098 | HZ1  | LYS | 159 | 14.443 | -22.365 | -21.787 | 1.00 | 0.00  |
| ATOM | 6099 | HZ2  | LYS | 159 | 14.661 | -24.004 | -22.157 | 1.00 | 0.00  |
| ATOM | 6100 | HZ3  | LYS | 159 | 14.616 | -22.857 | -23.400 | 1.00 | 0.00  |
| ATOM | 6101 | N    | VAL | 160 | 16.979 | -19.427 | -17.586 | 1.00 | 28.27 |
| ATOM | 6102 | CA   | VAL | 160 | 17.584 | -18.118 | -17.717 | 1.00 | 27.22 |
| ATOM | 6103 | C    | VAL | 160 | 18.995 | -18.138 | -18.300 | 1.00 | 26.89 |
| ATOM | 6104 | O    | VAL | 160 | 19.783 | -19.056 | -18.042 | 1.00 | 26.21 |
| ATOM | 6105 | CB   | VAL | 160 | 17.579 | -17.352 | -16.365 | 1.00 | 26.37 |
| ATOM | 6106 | CG1  | VAL | 160 | 16.152 | -17.061 | -15.937 | 1.00 | 25.49 |
| ATOM | 6107 | CG2  | VAL | 160 | 18.309 | -18.145 | -15.285 | 1.00 | 25.91 |
| ATOM | 6108 | H    | VAL | 160 | 17.425 | -20.106 | -17.051 | 1.00 | 0.00  |
| ATOM | 6109 | N    | PRO | 161 | 19.289 | -17.165 | -19.177 | 1.00 | 26.61 |
| ATOM | 6110 | CA   | PRO | 161 | 20.592 | -17.028 | -19.824 | 1.00 | 26.53 |
| ATOM | 6111 | C    | PRO | 161 | 21.541 | -16.258 | -18.912 | 1.00 | 27.45 |
| ATOM | 6112 | O    | PRO | 161 | 21.225 | -15.153 | -18.465 | 1.00 | 28.05 |
| ATOM | 6113 | CB   | PRO | 161 | 20.255 | -16.212 | -21.069 | 1.00 | 26.69 |
| ATOM | 6114 | CG   | PRO | 161 | 19.180 | -15.299 | -20.582 | 1.00 | 24.96 |
| ATOM | 6115 | CD   | PRO | 161 | 18.309 | -16.234 | -19.774 | 1.00 | 26.06 |
| ATOM | 6116 | N    | ILE | 162 | 22.665 | -16.864 | -18.570 | 1.00 | 27.75 |
| ATOM | 6117 | CA   | ILE | 162 | 23.630 | -16.184 | -17.729 | 1.00 | 27.79 |
| ATOM | 6118 | C    | ILE | 162 | 24.371 | -15.185 | -18.607 | 1.00 | 29.32 |
| ATOM | 6119 | O    | ILE | 162 | 24.574 | -15.444 | -19.795 | 1.00 | 29.91 |
| ATOM | 6120 | CB   | ILE | 162 | 24.619 | -17.179 | -17.128 | 1.00 | 27.56 |
| ATOM | 6121 | CG1  | ILE | 162 | 23.909 | -18.033 | -16.087 | 1.00 | 28.94 |
| ATOM | 6122 | CG2  | ILE | 162 | 25.797 | -16.461 | -16.504 | 1.00 | 28.96 |
| ATOM | 6123 | H    | ILE | 162 | 22.834 | -17.778 | -18.867 | 1.00 | 0.00  |
| ATOM | 6124 | CD   | ILE | 162 | 24.851 | -18.804 | -15.197 | 1.00 | 30.81 |
| ATOM | 6125 | N    | MET | 163 | 24.695 | -14.017 | -18.062 | 1.00 | 30.79 |
| ATOM | 6126 | CA   | MET | 163 | 25.442 | -13.025 | -18.831 | 1.00 | 32.65 |
| ATOM | 6127 | C    | MET | 163 | 26.647 | -12.474 | -18.075 | 1.00 | 33.28 |
| ATOM | 6128 | O    | MET | 163 | 26.630 | -12.329 | -16.848 | 1.00 | 33.19 |
| ATOM | 6129 | CB   | MET | 163 | 24.548 | -11.900 | -19.361 | 1.00 | 33.77 |
| ATOM | 6130 | CG   | MET | 163 | 24.097 | -10.861 | -18.360 | 1.00 | 34.64 |
| ATOM | 6131 | SD   | MET | 163 | 23.301 | -9.518  | -19.261 | 1.00 | 35.59 |
| ATOM | 6132 | CE   | MET | 163 | 21.836 | -10.392 | -19.907 | 1.00 | 36.49 |
| ATOM | 6133 | H    | MET | 163 | 24.435 | -13.850 | -17.131 | 1.00 | 0.00  |
| ATOM | 6134 | N    | GLU | 164 | 27.700 | -12.190 | -18.834 | 1.00 | 34.37 |
| ATOM | 6135 | CA   | GLU | 164 | 28.962 | -11.699 | -18.299 | 1.00 | 34.87 |
| ATOM | 6136 | C    | GLU | 164 | 28.812 | -10.420 | -17.481 | 1.00 | 33.17 |
| ATOM | 6137 | O    | GLU | 164 | 28.137 | -9.478  | -17.898 | 1.00 | 33.20 |
| ATOM | 6138 | CB   | GLU | 164 | 29.955 | -11.513 | -19.451 | 1.00 | 37.78 |
| ATOM | 6139 | CG   | GLU | 164 | 31.407 | -11.771 | -19.083 | 1.00 | 42.81 |
| ATOM | 6140 | CD   | GLU | 164 | 32.102 | -10.534 | -18.541 | 1.00 | 46.15 |
| ATOM | 6141 | OE1  | GLU | 164 | 32.348 | -10.453 | -17.314 | 1.00 | 47.13 |
| ATOM | 6142 | OE2  | GLU | 164 | 32.398 | -9.627  | -19.349 | 1.00 | 47.50 |
| ATOM | 6143 | H    | GLU | 164 | 27.612 | -12.290 | -19.799 | 1.00 | 0.00  |
| ATOM | 6144 | N    | ASN | 165 | 29.470 | -10.397 | -16.324 | 1.00 | 31.91 |
| ATOM | 6145 | CA   | ASN | 165 | 29.433 | -9.268  | -15.392 | 1.00 | 30.92 |
| ATOM | 6146 | C    | ASN | 165 | 29.581 | -7.912  | -16.060 | 1.00 | 31.33 |
| ATOM | 6147 | O    | ASN | 165 | 28.853 | -6.976  | -15.752 | 1.00 | 31.17 |
| ATOM | 6148 | CB   | ASN | 165 | 30.531 | -9.407  | -14.329 | 1.00 | 29.99 |
| ATOM | 6149 | CG   | ASN | 165 | 30.052 | -10.101 | -13.060 | 1.00 | 29.08 |
| ATOM | 6150 | OD1  | ASN | 165 | 29.608 | -11.253 | -13.084 | 1.00 | 28.43 |
| ATOM | 6151 | ND2  | ASN | 165 | 30.182 | -9.413  | -11.937 | 1.00 | 29.03 |
| ATOM | 6152 | H    | ASN | 165 | 30.041 | -11.168 | -16.122 | 1.00 | 0.00  |
| ATOM | 6153 | HD21 | ASN | 165 | 30.572 | -8.511  | -11.948 | 1.00 | 0.00  |
| ATOM | 6154 | HD22 | ASN | 165 | 29.867 | -9.826  | -11.110 | 1.00 | 0.00  |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 6155 | N   | HIS | 166 | 30.518 | -7.807 | -16.989 | 1.00 | 32.40 |
| ATOM | 6156 | CA  | HIS | 166 | 30.757 | -6.544 | -17.665 | 1.00 | 33.70 |
| ATOM | 6157 | C   | HIS | 166 | 29.581 | -6.105 | -18.522 | 1.00 | 32.64 |
| ATOM | 6158 | O   | HIS | 166 | 29.161 | -4.954 | -18.449 | 1.00 | 33.42 |
| ATOM | 6159 | CB  | HIS | 166 | 32.064 | -6.628 | -18.430 | 1.00 | 38.28 |
| ATOM | 6160 | CG  | HIS | 166 | 33.186 | -7.156 | -17.591 | 1.00 | 45.08 |
| ATOM | 6161 | ND1 | HIS | 166 | 34.050 | -8.139 | -18.024 | 1.00 | 48.15 |
| ATOM | 6162 | CD2 | HIS | 166 | 33.531 | -6.895 | -16.306 | 1.00 | 46.84 |
| ATOM | 6163 | CE1 | HIS | 166 | 34.874 | -8.465 | -17.043 | 1.00 | 49.33 |
| ATOM | 6164 | NE2 | HIS | 166 | 34.580 | -7.725 | -15.989 | 1.00 | 48.48 |
| ATOM | 6165 | H   | HIS | 166 | 31.034 | -8.615 | -17.227 | 1.00 | 0.00  |
| ATOM | 6166 | HD1 | HIS | 166 | 33.982 | -8.621 | -18.884 | 1.00 | 0.00  |
| ATOM | 6167 | HE2 | HIS | 166 | 35.036 | -7.774 | -15.124 | 1.00 | 0.00  |
| ATOM | 6168 | N   | ILE | 167 | 29.003 | -7.030 | -19.275 | 1.00 | 30.67 |
| ATOM | 6169 | CA  | ILE | 167 | 27.840 | -6.715 | -20.098 | 1.00 | 29.12 |
| ATOM | 6170 | C   | ILE | 167 | 26.733 | -6.249 | -19.146 | 1.00 | 28.75 |
| ATOM | 6171 | O   | ILE | 167 | 26.059 | -5.245 | -19.381 | 1.00 | 29.01 |
| ATOM | 6172 | CB  | ILE | 167 | 27.350 | -7.973 | -20.872 | 1.00 | 28.84 |
| ATOM | 6173 | CG1 | ILE | 167 | 28.319 | -8.313 | -21.999 | 1.00 | 27.30 |
| ATOM | 6174 | CG2 | ILE | 167 | 25.958 | -7.753 | -21.448 | 1.00 | 28.44 |
| ATOM | 6175 | H   | ILE | 167 | 29.360 | -7.946 | -19.276 | 1.00 | 0.00  |
| ATOM | 6176 | CD  | ILE | 167 | 28.337 | -7.284 | -23.094 | 1.00 | 27.99 |
| ATOM | 6177 | N   | CYS | 168 | 26.589 | -6.975 | -18.046 | 1.00 | 28.45 |
| ATOM | 6178 | CA  | CYS | 168 | 25.581 | -6.687 | -17.036 | 1.00 | 29.22 |
| ATOM | 6179 | C   | CYS | 168 | 25.718 | -5.303 | -16.399 | 1.00 | 30.84 |
| ATOM | 6180 | O   | CYS | 168 | 24.728 | -4.577 | -16.260 | 1.00 | 32.38 |
| ATOM | 6181 | CB  | CYS | 168 | 25.636 | -7.758 | -15.957 | 1.00 | 28.37 |
| ATOM | 6182 | SG  | CYS | 168 | 24.312 | -7.650 | -14.729 | 1.00 | 26.91 |
| ATOM | 6183 | H   | CYS | 168 | 27.165 | -7.760 | -17.930 | 1.00 | 0.00  |
| ATOM | 6184 | N   | ASP | 169 | 26.938 | -4.949 | -16.001 | 1.00 | 30.44 |
| ATOM | 6185 | CA  | ASP | 169 | 27.228 | -3.655 | -15.383 | 1.00 | 28.55 |
| ATOM | 6186 | C   | ASP | 169 | 26.885 | -2.528 | -16.361 | 1.00 | 27.27 |
| ATOM | 6187 | O   | ASP | 169 | 26.285 | -1.526 | -15.979 | 1.00 | 26.35 |
| ATOM | 6188 | CB  | ASP | 169 | 28.708 | -3.599 | -14.996 | 1.00 | 30.58 |
| ATOM | 6189 | CG  | ASP | 169 | 29.033 | -2.449 | -14.060 | 1.00 | 32.32 |
| ATOM | 6190 | OD1 | ASP | 169 | 28.561 | -2.462 | -12.904 | 1.00 | 33.26 |
| ATOM | 6191 | OD2 | ASP | 169 | 29.796 | -1.544 | -14.464 | 1.00 | 32.34 |
| ATOM | 6192 | H   | ASP | 169 | 27.671 | -5.581 | -16.083 | 1.00 | 0.00  |
| ATOM | 6193 | N   | ALA | 170 | 27.248 | -2.709 | -17.630 | 1.00 | 26.35 |
| ATOM | 6194 | CA  | ALA | 170 | 26.956 | -1.722 | -18.665 | 1.00 | 25.15 |
| ATOM | 6195 | C   | ALA | 170 | 25.455 | -1.511 | -18.703 | 1.00 | 23.75 |
| ATOM | 6196 | O   | ALA | 170 | 24.973 | -0.384 | -18.631 | 1.00 | 24.34 |
| ATOM | 6197 | CB  | ALA | 170 | 27.445 | -2.208 | -20.014 | 1.00 | 26.07 |
| ATOM | 6198 | H   | ALA | 170 | 27.761 | -3.514 | -17.857 | 1.00 | 0.00  |
| ATOM | 6199 | N   | LYS | 171 | 24.725 | -2.611 | -18.797 | 1.00 | 22.46 |
| ATOM | 6200 | CA  | LYS | 171 | 23.273 | -2.575 | -18.816 | 1.00 | 22.07 |
| ATOM | 6201 | C   | LYS | 171 | 22.772 | -1.712 | -17.663 | 1.00 | 20.74 |
| ATOM | 6202 | O   | LYS | 171 | 22.021 | -0.762 | -17.870 | 1.00 | 20.15 |
| ATOM | 6203 | CB  | LYS | 171 | 22.721 | -3.983 | -18.634 | 1.00 | 23.88 |
| ATOM | 6204 | CG  | LYS | 171 | 23.183 | -4.966 | -19.665 | 1.00 | 24.76 |
| ATOM | 6205 | CD  | LYS | 171 | 22.430 | -4.771 | -20.949 | 1.00 | 27.86 |
| ATOM | 6206 | CE  | LYS | 171 | 22.424 | -6.060 | -21.746 | 1.00 | 31.18 |
| ATOM | 6207 | NZ  | LYS | 171 | 21.977 | -7.227 | -20.908 | 1.00 | 32.72 |
| ATOM | 6208 | H   | LYS | 171 | 25.193 | -3.465 | -18.876 | 1.00 | 0.00  |
| ATOM | 6209 | HZ1 | LYS | 171 | 21.027 | -7.074 | -20.525 | 1.00 | 0.00  |
| ATOM | 6210 | HZ2 | LYS | 171 | 22.649 | -7.380 | -20.128 | 1.00 | 0.00  |
| ATOM | 6211 | HZ3 | LYS | 171 | 21.969 | -8.081 | -21.504 | 1.00 | 0.00  |
| ATOM | 6212 | N   | TYR | 172 | 23.220 | -2.035 | -16.454 | 1.00 | 19.02 |
| ATOM | 6213 | CA  | TYR | 172 | 22.816 | -1.301 | -15.266 | 1.00 | 17.28 |
| ATOM | 6214 | C   | TYR | 172 | 23.127 | 0.195  | -15.299 | 1.00 | 17.38 |
| ATOM | 6215 | O   | TYR | 172 | 22.454 | 0.982  | -14.630 | 1.00 | 18.78 |
| ATOM | 6216 | CB  | TYR | 172 | 23.362 | -1.969 | -13.998 | 1.00 | 15.58 |
| ATOM | 6217 | CG  | TYR | 172 | 22.363 | -2.927 | -13.395 | 1.00 | 16.07 |

|      |      |     |     |      |        |        |         |      |       |
|------|------|-----|-----|------|--------|--------|---------|------|-------|
| ATOM | 6218 | CD1 | TYR | 172  | 22.124 | -4.172 | -13.976 | 1.00 | 16.89 |
| ATOM | 6219 | CD2 | TYR | 172  | 21.570 | -2.548 | -12.311 | 1.00 | 16.35 |
| ATOM | 6220 | CE1 | TYR | 172  | 21.108 | -5.013 | -13.498 | 1.00 | 15.96 |
| ATOM | 6221 | CE2 | TYR | 172  | 20.552 | -3.381 | -11.829 | 1.00 | 15.73 |
| ATOM | 6222 | CZ  | TYR | 172  | 20.328 | -4.607 | -12.431 | 1.00 | 15.06 |
| ATOM | 6223 | OH  | TYR | 172  | 19.309 | -5.411 | -11.985 | 1.00 | 14.10 |
| ATOM | 6224 | H   | TYR | 172  | 23.820 | -2.807 | -16.363 | 1.00 | 0.00  |
| ATOM | 6225 | HH  | TYR | 172  | 19.348 | -6.256 | -12.442 | 1.00 | 0.00  |
| ATOM | 6226 | N   | HIS | 173  | 24.110 | 0.596  | -16.100 | 1.00 | 16.05 |
| ATOM | 6227 | CA  | HIS | 173  | 24.460 | 2.013  | -16.206 | 1.00 | 14.57 |
| ATOM | 6228 | C   | HIS | 173  | 23.586 | 2.773  | -17.207 | 1.00 | 15.85 |
| ATOM | 6229 | O   | HIS | 173  | 23.480 | 4.007  | -17.132 | 1.00 | 17.58 |
| ATOM | 6230 | CB  | HIS | 173  | 25.934 | 2.188  | -16.553 | 1.00 | 10.64 |
| ATOM | 6231 | CG  | HIS | 173  | 26.851 | 1.918  | -15.409 | 1.00 | 8.84  |
| ATOM | 6232 | ND1 | HIS | 173  | 27.338 | 2.917  | -14.594 | 1.00 | 9.45  |
| ATOM | 6233 | CD2 | HIS | 173  | 27.358 | 0.760  | -14.928 | 1.00 | 8.00  |
| ATOM | 6234 | CE1 | HIS | 173  | 28.106 | 2.384  | -13.659 | 1.00 | 9.58  |
| ATOM | 6235 | NE2 | HIS | 173  | 28.135 | 1.076  | -13.841 | 1.00 | 8.41  |
| ATOM | 6236 | H   | HIS | 173  | 24.601 | -0.080 | -16.615 | 1.00 | 0.00  |
| ATOM | 6237 | HD1 | HIS | 173  | 27.189 | 3.891  | -14.673 | 1.00 | 0.00  |
| ATOM | 6238 | HE2 | HIS | 173  | 28.689 | 0.434  | -13.341 | 1.00 | 0.00  |
| ATOM | 6239 | N   | LEU | 173A | 22.973 | 2.045  | -18.142 | 1.00 | 14.07 |
| ATOM | 6240 | CA  | LEU | 173A | 22.105 | 2.648  | -19.149 | 1.00 | 11.77 |
| ATOM | 6241 | C   | LEU | 173A | 20.912 | 3.293  | -18.459 | 1.00 | 13.24 |
| ATOM | 6242 | O   | LEU | 173A | 20.237 | 2.670  | -17.640 | 1.00 | 14.73 |
| ATOM | 6243 | CB  | LEU | 173A | 21.613 | 1.587  | -20.130 | 1.00 | 9.85  |
| ATOM | 6244 | CG  | LEU | 173A | 22.680 | 0.801  | -20.894 | 1.00 | 10.26 |
| ATOM | 6245 | CD1 | LEU | 173A | 22.073 | -0.397 | -21.583 | 1.00 | 9.89  |
| ATOM | 6246 | CD2 | LEU | 173A | 23.349 | 1.691  | -21.907 | 1.00 | 11.81 |
| ATOM | 6247 | H   | LEU | 173A | 23.103 | 1.071  | -18.146 | 1.00 | 0.00  |
| ATOM | 6248 | N   | GLY | 173B | 20.677 | 4.563  | -18.748 | 1.00 | 15.00 |
| ATOM | 6249 | CA  | GLY | 173B | 19.555 | 5.246  | -18.138 | 1.00 | 18.48 |
| ATOM | 6250 | C   | GLY | 173B | 19.760 | 5.596  | -16.674 | 1.00 | 22.14 |
| ATOM | 6251 | O   | GLY | 173B | 18.801 | 5.926  | -15.978 | 1.00 | 24.14 |
| ATOM | 6252 | H   | GLY | 173B | 21.284 | 5.029  | -19.353 | 1.00 | 0.00  |
| ATOM | 6253 | N   | ALA | 173C | 21.002 | 5.541  | -16.203 | 1.00 | 22.27 |
| ATOM | 6254 | CA  | ALA | 173C | 21.306 | 5.882  | -14.821 | 1.00 | 21.54 |
| ATOM | 6255 | C   | ALA | 173C | 22.427 | 6.914  | -14.831 | 1.00 | 21.93 |
| ATOM | 6256 | O   | ALA | 173C | 23.227 | 6.955  | -15.774 | 1.00 | 22.84 |
| ATOM | 6257 | CB  | ALA | 173C | 21.735 | 4.638  | -14.059 | 1.00 | 21.95 |
| ATOM | 6258 | H   | ALA | 173C | 21.765 | 5.255  | -16.747 | 1.00 | 0.00  |
| ATOM | 6259 | N   | TYR | 173D | 22.463 | 7.757  | -13.798 | 1.00 | 21.41 |
| ATOM | 6260 | CA  | TYR | 173D | 23.479 | 8.810  | -13.641 | 1.00 | 20.23 |
| ATOM | 6261 | C   | TYR | 173D | 24.840 | 8.274  | -13.163 | 1.00 | 19.62 |
| ATOM | 6262 | O   | TYR | 173D | 25.873 | 8.907  | -13.374 | 1.00 | 18.00 |
| ATOM | 6263 | CB  | TYR | 173D | 23.001 | 9.859  | -12.628 | 1.00 | 20.30 |
| ATOM | 6264 | CG  | TYR | 173D | 21.779 | 10.658 | -13.028 | 1.00 | 19.63 |
| ATOM | 6265 | CD1 | TYR | 173D | 21.840 | 11.596 | -14.055 | 1.00 | 18.76 |
| ATOM | 6266 | CD2 | TYR | 173D | 20.575 | 10.512 | -12.348 | 1.00 | 20.08 |
| ATOM | 6267 | CE1 | TYR | 173D | 20.739 | 12.364 | -14.391 | 1.00 | 18.98 |
| ATOM | 6268 | CE2 | TYR | 173D | 19.467 | 11.279 | -12.678 | 1.00 | 19.99 |
| ATOM | 6269 | CZ  | TYR | 173D | 19.558 | 12.201 | -13.699 | 1.00 | 19.88 |
| ATOM | 6270 | OH  | TYR | 173D | 18.467 | 12.969 | -14.021 | 1.00 | 22.48 |
| ATOM | 6271 | H   | TYR | 173D | 21.766 | 7.652  | -13.138 | 1.00 | 0.00  |
| ATOM | 6272 | HH  | TYR | 173D | 17.822 | 12.842 | -13.317 | 1.00 | 0.00  |
| ATOM | 6273 | N   | THR | 173E | 24.813 | 7.139  | -12.467 | 1.00 | 20.33 |
| ATOM | 6274 | CA  | THR | 173E | 26.006 | 6.500  | -11.932 | 1.00 | 20.71 |
| ATOM | 6275 | C   | THR | 173E | 27.124 | 6.421  | -12.955 | 1.00 | 23.06 |
| ATOM | 6276 | O   | THR | 173E | 26.953 | 5.848  | -14.040 | 1.00 | 24.05 |
| ATOM | 6277 | CB  | THR | 173E | 25.700 | 5.073  | -11.476 | 1.00 | 19.83 |
| ATOM | 6278 | OG1 | THR | 173E | 24.477 | 5.060  | -10.732 | 1.00 | 19.44 |
| ATOM | 6279 | CG2 | THR | 173E | 26.822 | 4.549  | -10.607 | 1.00 | 19.36 |
| ATOM | 6280 | H   | THR | 173E | 23.956 | 6.720  | -12.273 | 1.00 | 0.00  |

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|      |      |      |     |      |        |        |         |      |       |
|------|------|------|-----|------|--------|--------|---------|------|-------|
| ATOM | 6281 | HG1  | THR | 173E | 23.715 | 4.967  | -11.309 | 1.00 | 0.00  |
| ATOM | 6282 | N    | GLY | 173F | 28.286 | 6.943  | -12.577 | 1.00 | 24.83 |
| ATOM | 6283 | CA   | GLY | 173F | 29.440 | 6.941  | -13.460 | 1.00 | 27.60 |
| ATOM | 6284 | C    | GLY | 173F | 29.882 | 5.561  | -13.911 | 1.00 | 29.17 |
| ATOM | 6285 | O    | GLY | 173F | 29.857 | 4.599  | -13.139 | 1.00 | 28.51 |
| ATOM | 6286 | H    | GLY | 173F | 28.353 | 7.307  | -11.681 | 1.00 | 0.00  |
| ATOM | 6287 | N    | ASP | 173G | 30.303 | 5.468  | -15.166 | 1.00 | 31.24 |
| ATOM | 6288 | CA   | ASP | 173G | 30.746 | 4.205  | -15.729 | 1.00 | 33.43 |
| ATOM | 6289 | C    | ASP | 173G | 31.799 | 3.534  | -14.871 | 1.00 | 34.71 |
| ATOM | 6290 | O    | ASP | 173G | 31.821 | 2.308  | -14.759 | 1.00 | 36.55 |
| ATOM | 6291 | CB   | ASP | 173G | 31.272 | 4.405  | -17.148 | 1.00 | 34.43 |
| ATOM | 6292 | CG   | ASP | 173G | 30.163 | 4.665  | -18.144 | 1.00 | 36.11 |
| ATOM | 6293 | OD1  | ASP | 173G | 29.269 | 3.803  | -18.274 | 1.00 | 37.29 |
| ATOM | 6294 | OD2  | ASP | 173G | 30.175 | 5.734  | -18.789 | 1.00 | 36.29 |
| ATOM | 6295 | H    | ASP | 173G | 30.290 | 6.246  | -15.758 | 1.00 | 0.00  |
| ATOM | 6296 | N    | ASP | 173H | 32.645 | 4.337  | -14.234 | 1.00 | 34.50 |
| ATOM | 6297 | CA   | ASP | 173H | 33.706 | 3.803  | -13.390 | 1.00 | 35.01 |
| ATOM | 6298 | C    | ASP | 173H | 33.194 | 3.142  | -12.121 | 1.00 | 32.60 |
| ATOM | 6299 | O    | ASP | 173H | 33.854 | 2.265  | -11.562 | 1.00 | 33.16 |
| ATOM | 6300 | CB   | ASP | 173H | 34.736 | 4.886  | -13.070 | 1.00 | 40.25 |
| ATOM | 6301 | CG   | ASP | 173H | 35.561 | 5.281  | -14.292 | 1.00 | 45.56 |
| ATOM | 6302 | OD1  | ASP | 173H | 36.179 | 4.388  | -14.919 | 1.00 | 47.19 |
| ATOM | 6303 | OD2  | ASP | 173H | 35.557 | 6.475  | -14.670 | 1.00 | 48.34 |
| ATOM | 6304 | H    | ASP | 173H | 32.567 | 5.306  | -14.336 | 1.00 | 0.00  |
| ATOM | 6305 | N    | VAL | 173I | 31.995 | 3.517  | -11.701 | 1.00 | 29.46 |
| ATOM | 6306 | CA   | VAL | 173I | 31.392 | 2.948  | -10.509 | 1.00 | 27.51 |
| ATOM | 6307 | C    | VAL | 173I | 30.876 | 1.555  | -10.833 | 1.00 | 27.15 |
| ATOM | 6308 | O    | VAL | 173I | 30.244 | 1.349  | -11.871 | 1.00 | 27.25 |
| ATOM | 6309 | CB   | VAL | 173I | 30.220 | 3.801  | -10.022 | 1.00 | 28.53 |
| ATOM | 6310 | CG1  | VAL | 173I | 29.587 | 3.177  | -8.792  | 1.00 | 29.23 |
| ATOM | 6311 | CG2  | VAL | 173I | 30.690 | 5.215  | -9.724  | 1.00 | 29.26 |
| ATOM | 6312 | H    | VAL | 173I | 31.480 | 4.166  | -12.212 | 1.00 | 0.00  |
| ATOM | 6313 | N    | ARG | 174  | 31.162 | 0.602  | -9.949  | 1.00 | 26.56 |
| ATOM | 6314 | CA   | ARG | 174  | 30.741 | -0.781 | -10.126 | 1.00 | 25.40 |
| ATOM | 6315 | C    | ARG | 174  | 29.400 | -1.036 | -9.458  | 1.00 | 24.29 |
| ATOM | 6316 | O    | ARG | 174  | 29.270 | -0.899 | -8.238  | 1.00 | 23.86 |
| ATOM | 6317 | CB   | ARG | 174  | 31.784 | -1.729 | -9.535  | 1.00 | 27.85 |
| ATOM | 6318 | CG   | ARG | 174  | 31.866 | -3.094 | -10.204 | 1.00 | 30.55 |
| ATOM | 6319 | CD   | ARG | 174  | 32.704 | -3.042 | -11.473 | 1.00 | 34.47 |
| ATOM | 6320 | NE   | ARG | 174  | 32.139 | -2.146 | -12.485 | 1.00 | 40.01 |
| ATOM | 6321 | CZ   | ARG | 174  | 32.562 | -0.903 | -12.731 | 1.00 | 41.74 |
| ATOM | 6322 | NH1  | ARG | 174  | 33.569 | -0.378 | -12.036 | 1.00 | 41.34 |
| ATOM | 6323 | NH2  | ARG | 174  | 31.967 | -0.184 | -13.676 | 1.00 | 43.55 |
| ATOM | 6324 | H    | ARG | 174  | 31.649 | 0.845  | -9.137  | 1.00 | 0.00  |
| ATOM | 6325 | HE   | ARG | 174  | 31.366 | -2.490 | -13.008 | 1.00 | 0.00  |
| ATOM | 6326 | HH11 | ARG | 174  | 34.041 | -0.908 | -11.335 | 1.00 | 0.00  |
| ATOM | 6327 | HH12 | ARG | 174  | 33.904 | 0.565  | -12.183 | 1.00 | 0.00  |
| ATOM | 6328 | HH21 | ARG | 174  | 31.198 | -0.600 | -14.168 | 1.00 | 0.00  |
| ATOM | 6329 | HH22 | ARG | 174  | 32.159 | 0.760  | -13.960 | 1.00 | 0.00  |
| ATOM | 6330 | N    | ILE | 175  | 28.406 | -1.395 | -10.263 | 1.00 | 22.92 |
| ATOM | 6331 | CA   | ILE | 175  | 27.073 | -1.689 | -9.762  | 1.00 | 21.26 |
| ATOM | 6332 | C    | ILE | 175  | 27.008 | -3.183 | -9.441  | 1.00 | 21.48 |
| ATOM | 6333 | O    | ILE | 175  | 26.802 | -3.571 | -8.284  | 1.00 | 21.74 |
| ATOM | 6334 | CB   | ILE | 175  | 25.997 | -1.280 | -10.788 | 1.00 | 19.49 |
| ATOM | 6335 | CG1  | ILE | 175  | 26.045 | 0.236  | -10.992 | 1.00 | 19.32 |
| ATOM | 6336 | CG2  | ILE | 175  | 24.609 | -1.699 | -10.312 | 1.00 | 20.43 |
| ATOM | 6337 | H    | ILE | 175  | 28.573 | -1.524 | -11.216 | 1.00 | 0.00  |
| ATOM | 6338 | CD   | ILE | 175  | 25.037 | 0.767  | -11.987 | 1.00 | 19.59 |
| ATOM | 6339 | N    | VAL | 176  | 27.211 | -4.016 | -10.453 | 1.00 | 20.59 |
| ATOM | 6340 | CA   | VAL | 176  | 27.200 | -5.454 | -10.243 | 1.00 | 22.12 |
| ATOM | 6341 | C    | VAL | 176  | 28.625 | -5.879 | -9.866  | 1.00 | 23.64 |
| ATOM | 6342 | O    | VAL | 176  | 29.525 | -5.942 | -10.712 | 1.00 | 24.09 |
| ATOM | 6343 | CB   | VAL | 176  | 26.638 | -6.229 | -11.484 | 1.00 | 22.49 |

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|      |      |      |     |     |        |         |         |      |       |
|------|------|------|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6344 | CG1  | VAL | 176 | 27.286 | -5.768  | -12.752 | 1.00 | 23.91 |
| ATOM | 6345 | CG2  | VAL | 176 | 26.833 | -7.725  | -11.320 | 1.00 | 22.89 |
| ATOM | 6346 | H    | VAL | 176 | 27.448 | -3.639  | -11.332 | 1.00 | 0.00  |
| ATOM | 6347 | N    | ARG | 177 | 28.825 | -6.104  | -8.570  | 1.00 | 24.34 |
| ATOM | 6348 | CA   | ARG | 177 | 30.121 | -6.492  | -8.020  | 1.00 | 24.78 |
| ATOM | 6349 | C    | ARG | 177 | 30.582 | -7.911  | -8.366  | 1.00 | 24.94 |
| ATOM | 6350 | O    | ARG | 177 | 29.796 | -8.735  | -8.825  | 1.00 | 26.22 |
| ATOM | 6351 | CB   | ARG | 177 | 30.113 | -6.301  | -6.504  | 1.00 | 27.87 |
| ATOM | 6352 | CG   | ARG | 177 | 30.020 | -4.850  | -6.053  | 1.00 | 32.78 |
| ATOM | 6353 | CD   | ARG | 177 | 28.587 | -4.393  | -5.807  | 1.00 | 37.25 |
| ATOM | 6354 | NE   | ARG | 177 | 28.466 | -2.933  | -5.810  | 1.00 | 41.21 |
| ATOM | 6355 | CZ   | ARG | 177 | 28.990 | -2.118  | -4.892  | 1.00 | 41.76 |
| ATOM | 6356 | NH1  | ARG | 177 | 29.678 | -2.606  | -3.863  | 1.00 | 42.08 |
| ATOM | 6357 | NH2  | ARG | 177 | 28.847 | -0.805  | -5.017  | 1.00 | 42.71 |
| ATOM | 6358 | H    | ARG | 177 | 28.055 | -6.018  | -7.971  | 1.00 | 0.00  |
| ATOM | 6359 | HE   | ARG | 177 | 27.922 | -2.596  | -6.568  | 1.00 | 0.00  |
| ATOM | 6360 | HH11 | ARG | 177 | 29.751 | -3.605  | -3.754  | 1.00 | 0.00  |
| ATOM | 6361 | HH12 | ARG | 177 | 30.087 | -2.033  | -3.162  | 1.00 | 0.00  |
| ATOM | 6362 | HH21 | ARG | 177 | 28.339 | -0.453  | -5.814  | 1.00 | 0.00  |
| ATOM | 6363 | HH22 | ARG | 177 | 29.173 | -0.127  | -4.371  | 1.00 | 0.00  |
| ATOM | 6364 | N    | ASP | 178 | 31.854 | -8.195  | -8.097  | 1.00 | 24.59 |
| ATOM | 6365 | CA   | ASP | 178 | 32.465 | -9.500  | -8.373  | 1.00 | 23.86 |
| ATOM | 6366 | C    | ASP | 178 | 31.832 | -10.745 | -7.727  | 1.00 | 22.44 |
| ATOM | 6367 | O    | ASP | 178 | 32.092 | -11.872 | -8.163  | 1.00 | 23.36 |
| ATOM | 6368 | CB   | ASP | 178 | 33.963 | -9.452  | -8.038  | 1.00 | 25.64 |
| ATOM | 6369 | CG   | ASP | 178 | 34.820 | -8.997  | -9.211  | 1.00 | 28.30 |
| ATOM | 6370 | OD1  | ASP | 178 | 35.912 | -9.581  | -9.411  | 1.00 | 28.87 |
| ATOM | 6371 | OD2  | ASP | 178 | 34.420 | -8.059  | -9.939  | 1.00 | 29.64 |
| ATOM | 6372 | H    | ASP | 178 | 32.455 | -7.517  | -7.728  | 1.00 | 0.00  |
| ATOM | 6373 | N    | ASP | 179 | 31.032 | -10.564 | -6.682  | 1.00 | 19.92 |
| ATOM | 6374 | CA   | ASP | 179 | 30.385 | -11.699 | -6.024  | 1.00 | 18.90 |
| ATOM | 6375 | C    | ASP | 179 | 28.914 | -11.827 | -6.426  | 1.00 | 19.64 |
| ATOM | 6376 | O    | ASP | 179 | 28.108 | -12.441 | -5.724  | 1.00 | 20.69 |
| ATOM | 6377 | CB   | ASP | 179 | 30.511 | -11.592 | -4.503  | 1.00 | 18.24 |
| ATOM | 6378 | CG   | ASP | 179 | 29.754 | -10.415 | -3.932  | 1.00 | 18.83 |
| ATOM | 6379 | OD1  | ASP | 179 | 29.864 | -9.303  | -4.489  | 1.00 | 20.67 |
| ATOM | 6380 | OD2  | ASP | 179 | 29.052 | -10.589 | -2.918  | 1.00 | 19.22 |
| ATOM | 6381 | H    | ASP | 179 | 30.867 | -9.676  | -6.294  | 1.00 | 0.00  |
| ATOM | 6382 | N    | MET | 180 | 28.580 | -11.286 | -7.590  | 1.00 | 19.25 |
| ATOM | 6383 | CA   | MET | 180 | 27.220 | -11.334 | -8.101  | 1.00 | 19.16 |
| ATOM | 6384 | C    | MET | 180 | 27.245 | -11.930 | -9.497  | 1.00 | 20.32 |
| ATOM | 6385 | O    | MET | 180 | 28.267 | -11.873 | -10.177 | 1.00 | 21.17 |
| ATOM | 6386 | CB   | MET | 180 | 26.636 | -9.921  | -8.170  | 1.00 | 19.27 |
| ATOM | 6387 | CG   | MET | 180 | 26.607 | -9.183  | -6.844  | 1.00 | 17.95 |
| ATOM | 6388 | SD   | MET | 180 | 26.288 | -7.431  | -7.077  | 1.00 | 16.87 |
| ATOM | 6389 | CE   | MET | 180 | 26.312 | -6.863  | -5.403  | 1.00 | 17.35 |
| ATOM | 6390 | H    | MET | 180 | 29.243 | -10.800 | -8.121  | 1.00 | 0.00  |
| ATOM | 6391 | N    | LEU | 181 | 26.115 | -12.482 | -9.921  | 1.00 | 22.07 |
| ATOM | 6392 | CA   | LEU | 181 | 25.967 | -13.098 | -11.236 | 1.00 | 23.42 |
| ATOM | 6393 | C    | LEU | 181 | 24.659 | -12.593 | -11.841 | 1.00 | 24.89 |
| ATOM | 6394 | O    | LEU | 181 | 23.673 | -12.409 | -11.125 | 1.00 | 26.40 |
| ATOM | 6395 | CB   | LEU | 181 | 25.928 | -14.622 | -11.083 | 1.00 | 23.48 |
| ATOM | 6396 | CG   | LEU | 181 | 25.744 | -15.515 | -12.315 | 1.00 | 25.81 |
| ATOM | 6397 | CD1  | LEU | 181 | 26.271 | -16.911 | -12.000 | 1.00 | 26.64 |
| ATOM | 6398 | CD2  | LEU | 181 | 24.283 | -15.578 | -12.755 | 1.00 | 25.91 |
| ATOM | 6399 | H    | LEU | 181 | 25.345 | -12.478 | -9.324  | 1.00 | 0.00  |
| ATOM | 6400 | N    | CYS | 182 | 24.634 | -12.389 | -13.151 | 1.00 | 24.20 |
| ATOM | 6401 | CA   | CYS | 182 | 23.426 | -11.898 | -13.794 | 1.00 | 24.34 |
| ATOM | 6402 | C    | CYS | 182 | 22.797 | -12.974 | -14.666 | 1.00 | 25.33 |
| ATOM | 6403 | O    | CYS | 182 | 23.502 | -13.784 | -15.269 | 1.00 | 26.32 |
| ATOM | 6404 | CB   | CYS | 182 | 23.742 | -10.648 | -14.621 | 1.00 | 24.83 |
| ATOM | 6405 | SG   | CYS | 182 | 24.561 | -9.347  | -13.647 | 1.00 | 27.72 |
| ATOM | 6406 | H    | CYS | 182 | 25.411 | -12.576 | -13.711 | 1.00 | 0.00  |

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|      |      |      |     |     |        |         |         |      |       |
|------|------|------|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6407 | N    | ALA | 183 | 21.470 | -12.990 | -14.712 | 1.00 | 25.85 |
| ATOM | 6408 | CA   | ALA | 183 | 20.729 | -13.956 | -15.519 | 1.00 | 26.27 |
| ATOM | 6409 | C    | ALA | 183 | 19.293 | -13.487 | -15.698 | 1.00 | 27.01 |
| ATOM | 6410 | O    | ALA | 183 | 18.693 | -12.933 | -14.778 | 1.00 | 27.47 |
| ATOM | 6411 | CB   | ALA | 183 | 20.749 | -15.328 | -14.861 | 1.00 | 26.34 |
| ATOM | 6412 | H    | ALA | 183 | 20.960 | -12.361 | -14.149 | 1.00 | 0.00  |
| ATOM | 6413 | N    | GLY | 184 | 18.761 | -13.674 | -16.900 | 1.00 | 27.29 |
| ATOM | 6414 | CA   | GLY | 184 | 17.394 | -13.275 | -17.172 | 1.00 | 28.10 |
| ATOM | 6415 | C    | GLY | 184 | 17.299 | -12.258 | -18.286 | 1.00 | 29.73 |
| ATOM | 6416 | O    | GLY | 184 | 18.287 | -11.976 | -18.962 | 1.00 | 30.38 |
| ATOM | 6417 | H    | GLY | 184 | 19.344 | -14.026 | -17.609 | 1.00 | 0.00  |
| ATOM | 6418 | N    | ASN | 185 | 16.099 | -11.730 | -18.496 | 1.00 | 31.48 |
| ATOM | 6419 | CA   | ASN | 185 | 15.841 | -10.733 | -19.528 | 1.00 | 33.77 |
| ATOM | 6420 | C    | ASN | 185 | 14.380 | -10.297 | -19.487 | 1.00 | 36.43 |
| ATOM | 6421 | O    | ASN | 185 | 13.611 | -10.783 | -18.657 | 1.00 | 38.67 |
| ATOM | 6422 | CB   | ASN | 185 | 16.196 | -11.271 | -20.918 | 1.00 | 32.16 |
| ATOM | 6423 | CG   | ASN | 185 | 15.516 | -12.575 | -21.225 | 1.00 | 31.74 |
| ATOM | 6424 | OD1  | ASN | 185 | 14.300 | -12.635 | -21.390 | 1.00 | 31.49 |
| ATOM | 6425 | ND2  | ASN | 185 | 16.298 | -13.630 | -21.324 | 1.00 | 32.97 |
| ATOM | 6426 | H    | ASN | 185 | 15.356 | -12.019 | -17.925 | 1.00 | 0.00  |
| ATOM | 6427 | HD21 | ASN | 185 | 17.258 | -13.440 | -21.191 | 1.00 | 0.00  |
| ATOM | 6428 | HD22 | ASN | 185 | 15.927 | -14.511 | -21.488 | 1.00 | 0.00  |
| ATOM | 6429 | N    | THR | 186 | 13.998 | -9.429  | -20.423 | 1.00 | 37.10 |
| ATOM | 6430 | CA   | THR | 186 | 12.641 | -8.885  | -20.521 | 1.00 | 37.46 |
| ATOM | 6431 | C    | THR | 186 | 11.484 | -9.886  | -20.613 | 1.00 | 38.35 |
| ATOM | 6432 | O    | THR | 186 | 10.318 | -9.485  | -20.643 | 1.00 | 39.07 |
| ATOM | 6433 | CB   | THR | 186 | 12.537 | -7.887  | -21.700 | 1.00 | 36.60 |
| ATOM | 6434 | OG1  | THR | 186 | 13.232 | -8.411  | -22.840 | 1.00 | 36.52 |
| ATOM | 6435 | CG2  | THR | 186 | 13.151 | -6.560  | -21.323 | 1.00 | 36.21 |
| ATOM | 6436 | H    | THR | 186 | 14.628 | -9.122  | -21.102 | 1.00 | 0.00  |
| ATOM | 6437 | HG1  | THR | 186 | 13.486 | -7.635  | -23.357 | 1.00 | 0.00  |
| ATOM | 6438 | N    | ARG | 187 | 11.803 | -11.175 | -20.691 | 1.00 | 38.27 |
| ATOM | 6439 | CA   | ARG | 187 | 10.783 | -12.208 | -20.777 | 1.00 | 38.12 |
| ATOM | 6440 | C    | ARG | 187 | 10.870 | -13.155 | -19.595 | 1.00 | 36.90 |
| ATOM | 6441 | O    | ARG | 187 | 9.848  | -13.555 | -19.041 | 1.00 | 37.32 |
| ATOM | 6442 | CB   | ARG | 187 | 10.931 | -12.993 | -22.081 | 1.00 | 40.52 |
| ATOM | 6443 | CG   | ARG | 187 | 10.638 | -12.183 | -23.340 | 1.00 | 44.95 |
| ATOM | 6444 | CD   | ARG | 187 | 11.503 | -12.646 | -24.500 | 1.00 | 49.28 |
| ATOM | 6445 | NE   | ARG | 187 | 12.925 | -12.450 | -24.207 | 1.00 | 53.89 |
| ATOM | 6446 | CZ   | ARG | 187 | 13.687 | -11.514 | -24.769 | 1.00 | 55.78 |
| ATOM | 6447 | NH1  | ARG | 187 | 13.162 | -10.679 | -25.661 | 1.00 | 57.86 |
| ATOM | 6448 | NH2  | ARG | 187 | 14.969 | -11.403 | -24.431 | 1.00 | 56.74 |
| ATOM | 6449 | H    | ARG | 187 | 12.729 | -11.465 | -20.697 | 1.00 | 0.00  |
| ATOM | 6450 | HE   | ARG | 187 | 13.291 | -13.011 | -23.486 | 1.00 | 0.00  |
| ATOM | 6451 | HH11 | ARG | 187 | 12.188 | -10.764 | -25.896 | 1.00 | 0.00  |
| ATOM | 6452 | HH12 | ARG | 187 | 13.681 | -9.958  | -26.122 | 1.00 | 0.00  |
| ATOM | 6453 | HH21 | ARG | 187 | 15.376 | -12.002 | -23.743 | 1.00 | 0.00  |
| ATOM | 6454 | HH22 | ARG | 187 | 15.563 | -10.706 | -24.842 | 1.00 | 0.00  |
| ATOM | 6455 | N    | ARG | 188 | 12.090 | -13.499 | -19.199 | 1.00 | 34.95 |
| ATOM | 6456 | CA   | ARG | 188 | 12.291 | -14.419 | -18.090 | 1.00 | 33.39 |
| ATOM | 6457 | C    | ARG | 188 | 13.176 | -13.830 | -17.011 | 1.00 | 31.05 |
| ATOM | 6458 | O    | ARG | 188 | 14.244 | -13.317 | -17.313 | 1.00 | 31.13 |
| ATOM | 6459 | CB   | ARG | 188 | 12.912 | -15.707 | -18.604 | 1.00 | 34.87 |
| ATOM | 6460 | CG   | ARG | 188 | 12.110 | -16.357 | -19.699 | 1.00 | 38.68 |
| ATOM | 6461 | CD   | ARG | 188 | 12.864 | -16.328 | -21.000 | 1.00 | 42.02 |
| ATOM | 6462 | NE   | ARG | 188 | 14.109 | -17.081 | -20.896 | 1.00 | 46.41 |
| ATOM | 6463 | CZ   | ARG | 188 | 14.997 | -17.211 | -21.876 | 1.00 | 49.05 |
| ATOM | 6464 | NH1  | ARG | 188 | 14.781 | -16.635 | -23.058 | 1.00 | 50.82 |
| ATOM | 6465 | NH2  | ARG | 188 | 16.101 | -17.923 | -21.669 | 1.00 | 49.87 |
| ATOM | 6466 | H    | ARG | 188 | 12.874 | -13.106 | -19.634 | 1.00 | 0.00  |
| ATOM | 6467 | HE   | ARG | 188 | 14.297 | -17.552 | -20.048 | 1.00 | 0.00  |
| ATOM | 6468 | HH11 | ARG | 188 | 13.927 | -16.133 | -23.209 | 1.00 | 0.00  |
| ATOM | 6469 | HH12 | ARG | 188 | 15.415 | -16.715 | -23.831 | 1.00 | 0.00  |

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|      |      |         |     |        |         |         |      |       |
|------|------|---------|-----|--------|---------|---------|------|-------|
| ATOM | 6470 | HH21ARG | 188 | 16.201 | -18.344 | -20.755 | 1.00 | 0.00  |
| ATOM | 6471 | HH22ARG | 188 | 16.826 | -18.065 | -22.347 | 1.00 | 0.00  |
| ATOM | 6472 | N ASP   | 189 | 12.742 | -13.939 | -15.757 | 1.00 | 28.76 |
| ATOM | 6473 | CA ASP  | 189 | 13.483 | -13.417 | -14.609 | 1.00 | 27.44 |
| ATOM | 6474 | C ASP   | 189 | 12.762 | -13.771 | -13.316 | 1.00 | 27.00 |
| ATOM | 6475 | O ASP   | 189 | 11.556 | -14.000 | -13.315 | 1.00 | 27.79 |
| ATOM | 6476 | CB ASP  | 189 | 13.617 | -11.889 | -14.697 | 1.00 | 27.38 |
| ATOM | 6477 | CG ASP  | 189 | 14.373 | -11.287 | -13.513 | 1.00 | 28.22 |
| ATOM | 6478 | OD1 ASP | 189 | 15.276 | -11.942 | -12.948 | 1.00 | 29.82 |
| ATOM | 6479 | OD2 ASP | 189 | 14.064 | -10.141 | -13.148 | 1.00 | 27.89 |
| ATOM | 6480 | H ASP   | 189 | 11.880 | -14.372 | -15.576 | 1.00 | 0.00  |
| ATOM | 6481 | N SER   | 190 | 13.515 | -13.882 | -12.230 | 1.00 | 26.45 |
| ATOM | 6482 | CA SER  | 190 | 12.943 | -14.172 | -10.920 | 1.00 | 25.89 |
| ATOM | 6483 | C SER   | 190 | 12.269 | -12.883 | -10.450 | 1.00 | 24.87 |
| ATOM | 6484 | O SER   | 190 | 12.551 | -11.807 | -10.984 | 1.00 | 25.54 |
| ATOM | 6485 | CB SER  | 190 | 14.043 | -14.597 | -9.945  | 1.00 | 26.77 |
| ATOM | 6486 | OG SER  | 190 | 15.255 | -13.894 | -10.197 | 1.00 | 29.26 |
| ATOM | 6487 | H SER   | 190 | 14.476 | -13.723 | -12.340 | 1.00 | 0.00  |
| ATOM | 6488 | HG SER  | 190 | 15.102 | -13.099 | -10.754 | 1.00 | 0.00  |
| ATOM | 6489 | N CYS   | 191 | 11.389 | -12.968 | -9.462  | 1.00 | 22.26 |
| ATOM | 6490 | CA CYS  | 191 | 10.710 | -11.773 | -9.001  | 1.00 | 20.67 |
| ATOM | 6491 | C CYS   | 191 | 10.534 | -11.759 | -7.493  | 1.00 | 20.52 |
| ATOM | 6492 | O CYS   | 191 | 11.106 | -12.585 | -6.786  | 1.00 | 19.52 |
| ATOM | 6493 | CB CYS  | 191 | 9.365  | -11.658 | -9.714  | 1.00 | 21.01 |
| ATOM | 6494 | SG CYS  | 191 | 8.594  | -10.013 | -9.644  | 1.00 | 21.77 |
| ATOM | 6495 | H CYS   | 191 | 11.174 | -13.827 | -9.039  | 1.00 | 0.00  |
| ATOM | 6496 | N GLN   | 192 | 9.777  | -10.788 | -6.992  | 1.00 | 22.70 |
| ATOM | 6497 | CA GLN  | 192 | 9.521  | -10.674 | -5.558  | 1.00 | 25.29 |
| ATOM | 6498 | C GLN   | 192 | 9.036  | -11.998 | -4.990  | 1.00 | 23.12 |
| ATOM | 6499 | O GLN   | 192 | 8.080  | -12.575 | -5.496  | 1.00 | 23.43 |
| ATOM | 6500 | CB GLN  | 192 | 8.456  | -9.606  | -5.281  | 1.00 | 31.39 |
| ATOM | 6501 | CG GLN  | 192 | 8.913  | -8.171  | -5.491  | 1.00 | 38.85 |
| ATOM | 6502 | CD GLN  | 192 | 10.047 | -7.782  | -4.560  | 1.00 | 43.04 |
| ATOM | 6503 | OE1 GLN | 192 | 10.028 | -8.106  | -3.363  | 1.00 | 45.01 |
| ATOM | 6504 | NE2 GLN | 192 | 11.052 | -7.096  | -5.107  | 1.00 | 43.76 |
| ATOM | 6505 | H GLN   | 192 | 9.359  | -10.141 | -7.598  | 1.00 | 0.00  |
| ATOM | 6506 | HE21GLN | 192 | 10.987 | -6.875  | -6.071  | 1.00 | 0.00  |
| ATOM | 6507 | HE22GLN | 192 | 11.810 | -6.842  | -4.549  | 1.00 | 0.00  |
| ATOM | 6508 | N GLY   | 193 | 9.689  | -12.470 | -3.938  | 1.00 | 20.67 |
| ATOM | 6509 | CA GLY  | 193 | 9.289  | -13.722 | -3.328  | 1.00 | 18.84 |
| ATOM | 6510 | C GLY   | 193 | 10.253 | -14.848 | -3.625  | 1.00 | 18.03 |
| ATOM | 6511 | O GLY   | 193 | 10.338 | -15.817 | -2.863  | 1.00 | 19.56 |
| ATOM | 6512 | H GLY   | 193 | 10.452 | -11.989 | -3.569  | 1.00 | 0.00  |
| ATOM | 6513 | N ASP   | 194 | 10.974 | -14.735 | -4.732  | 1.00 | 15.66 |
| ATOM | 6514 | CA ASP  | 194 | 11.927 | -15.761 | -5.101  | 1.00 | 15.59 |
| ATOM | 6515 | C ASP   | 194 | 13.253 | -15.573 | -4.377  | 1.00 | 16.52 |
| ATOM | 6516 | O ASP   | 194 | 14.087 | -16.476 | -4.350  | 1.00 | 16.73 |
| ATOM | 6517 | CB ASP  | 194 | 12.129 | -15.778 | -6.614  | 1.00 | 14.53 |
| ATOM | 6518 | CG ASP  | 194 | 10.874 | -16.191 | -7.366  | 1.00 | 13.66 |
| ATOM | 6519 | OD1 ASP | 194 | 10.233 | -17.183 | -6.972  | 1.00 | 13.44 |
| ATOM | 6520 | OD2 ASP | 194 | 10.520 | -15.521 | -8.357  | 1.00 | 12.82 |
| ATOM | 6521 | H ASP   | 194 | 10.881 | -13.985 | -5.355  | 1.00 | 0.00  |
| ATOM | 6522 | N SER   | 195 | 13.430 | -14.412 | -3.759  | 1.00 | 17.66 |
| ATOM | 6523 | CA SER  | 195 | 14.658 | -14.107 | -3.032  | 1.00 | 19.29 |
| ATOM | 6524 | C SER   | 195 | 15.060 | -15.277 | -2.167  | 1.00 | 19.20 |
| ATOM | 6525 | O SER   | 195 | 14.213 | -15.899 | -1.531  | 1.00 | 19.25 |
| ATOM | 6526 | CB SER  | 195 | 14.480 | -12.870 | -2.152  | 1.00 | 21.52 |
| ATOM | 6527 | OG SER  | 195 | 14.637 | -11.662 | -2.891  | 1.00 | 22.42 |
| ATOM | 6528 | H SER   | 195 | 12.720 | -13.758 | -3.820  | 1.00 | 0.00  |
| ATOM | 6529 | N GLY   | 196 | 16.347 | -15.598 | -2.180  | 1.00 | 19.52 |
| ATOM | 6530 | CA GLY  | 196 | 16.830 | -16.713 | -1.392  | 1.00 | 21.10 |
| ATOM | 6531 | C GLY   | 196 | 16.793 | -18.017 | -2.167  | 1.00 | 23.58 |
| ATOM | 6532 | O GLY   | 196 | 17.409 | -18.994 | -1.747  | 1.00 | 26.35 |

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|      |      |     |     |     |        |         |         |      |       |
|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6533 | H   | GLY | 196 | 16.943 | -15.056 | -2.736  | 1.00 | 0.00  |
| ATOM | 6534 | N   | GLY | 197 | 16.106 | -18.025 | -3.311  | 1.00 | 23.82 |
| ATOM | 6535 | CA  | GLY | 197 | 16.002 | -19.223 | -4.139  | 1.00 | 24.01 |
| ATOM | 6536 | C   | GLY | 197 | 17.256 | -19.562 | -4.928  | 1.00 | 24.11 |
| ATOM | 6537 | O   | GLY | 197 | 18.127 | -18.713 | -5.080  | 1.00 | 24.81 |
| ATOM | 6538 | H   | GLY | 197 | 15.625 | -17.241 | -3.623  | 1.00 | 0.00  |
| ATOM | 6539 | N   | PRO | 198 | 17.374 | -20.788 | -5.460  | 1.00 | 24.65 |
| ATOM | 6540 | CA  | PRO | 198 | 18.563 | -21.172 | -6.224  | 1.00 | 24.52 |
| ATOM | 6541 | C   | PRO | 198 | 18.539 | -20.972 | -7.727  | 1.00 | 24.82 |
| ATOM | 6542 | O   | PRO | 198 | 17.490 | -20.951 | -8.363  | 1.00 | 25.00 |
| ATOM | 6543 | CB  | PRO | 198 | 18.690 | -22.656 | -5.909  | 1.00 | 23.87 |
| ATOM | 6544 | CG  | PRO | 198 | 17.268 | -23.091 | -5.904  | 1.00 | 24.74 |
| ATOM | 6545 | CD  | PRO | 198 | 16.572 | -21.979 | -5.116  | 1.00 | 25.53 |
| ATOM | 6546 | N   | LEU | 199 | 19.734 | -20.821 | -8.275  | 1.00 | 25.70 |
| ATOM | 6547 | CA  | LEU | 199 | 19.941 | -20.701 | -9.704  | 1.00 | 26.54 |
| ATOM | 6548 | C   | LEU | 199 | 20.872 | -21.884 | -9.958  | 1.00 | 29.37 |
| ATOM | 6549 | O   | LEU | 199 | 22.048 | -21.848 | -9.576  | 1.00 | 31.12 |
| ATOM | 6550 | CB  | LEU | 199 | 20.646 | -19.394 | -10.057 | 1.00 | 24.78 |
| ATOM | 6551 | CG  | LEU | 199 | 21.342 | -19.373 | -11.428 | 1.00 | 24.32 |
| ATOM | 6552 | CD1 | LEU | 199 | 20.334 | -19.520 | -12.546 | 1.00 | 23.19 |
| ATOM | 6553 | CD2 | LEU | 199 | 22.137 | -18.092 | -11.598 | 1.00 | 24.50 |
| ATOM | 6554 | H   | LEU | 199 | 20.514 | -20.763 | -7.675  | 1.00 | 0.00  |
| ATOM | 6555 | N   | VAL | 200 | 20.322 | -22.959 | -10.511 | 1.00 | 29.76 |
| ATOM | 6556 | CA  | VAL | 200 | 21.096 | -24.159 | -10.796 | 1.00 | 28.82 |
| ATOM | 6557 | C   | VAL | 200 | 21.313 | -24.287 | -12.283 | 1.00 | 29.84 |
| ATOM | 6558 | O   | VAL | 200 | 20.422 | -23.967 | -13.071 | 1.00 | 29.99 |
| ATOM | 6559 | CB  | VAL | 200 | 20.373 | -25.415 | -10.315 | 1.00 | 28.66 |
| ATOM | 6560 | CG1 | VAL | 200 | 20.300 | -25.415 | -8.810  | 1.00 | 30.02 |
| ATOM | 6561 | CG2 | VAL | 200 | 18.971 | -25.472 | -10.898 | 1.00 | 28.90 |
| ATOM | 6562 | H   | VAL | 200 | 19.388 | -22.888 | -10.803 | 1.00 | 0.00  |
| ATOM | 6563 | N   | CYS | 201 | 22.498 | -24.747 | -12.663 | 1.00 | 31.53 |
| ATOM | 6564 | CA  | CYS | 201 | 22.832 | -24.929 | -14.073 | 1.00 | 33.30 |
| ATOM | 6565 | C   | CYS | 201 | 23.204 | -26.383 | -14.353 | 1.00 | 34.58 |
| ATOM | 6566 | O   | CYS | 201 | 23.748 | -27.079 | -13.487 | 1.00 | 33.37 |
| ATOM | 6567 | CB  | CYS | 201 | 23.986 | -24.011 | -14.473 | 1.00 | 33.64 |
| ATOM | 6568 | SG  | CYS | 201 | 23.714 | -22.241 | -14.150 | 1.00 | 33.75 |
| ATOM | 6569 | H   | CYS | 201 | 23.147 | -24.973 | -11.972 | 1.00 | 0.00  |
| ATOM | 6570 | N   | LYS | 202 | 22.852 | -26.847 | -15.546 | 1.00 | 37.19 |
| ATOM | 6571 | CA  | LYS | 202 | 23.141 | -28.209 | -15.977 | 1.00 | 41.17 |
| ATOM | 6572 | C   | LYS | 202 | 24.597 | -28.304 | -16.446 | 1.00 | 43.78 |
| ATOM | 6573 | O   | LYS | 202 | 24.894 | -28.170 | -17.638 | 1.00 | 44.36 |
| ATOM | 6574 | CB  | LYS | 202 | 22.170 | -28.598 | -17.100 | 1.00 | 42.84 |
| ATOM | 6575 | CG  | LYS | 202 | 22.556 | -29.821 | -17.921 | 1.00 | 45.62 |
| ATOM | 6576 | CD  | LYS | 202 | 22.537 | -31.089 | -17.106 | 1.00 | 48.05 |
| ATOM | 6577 | CE  | LYS | 202 | 21.135 | -31.416 | -16.636 | 1.00 | 50.09 |
| ATOM | 6578 | NZ  | LYS | 202 | 21.097 | -32.727 | -15.932 | 1.00 | 52.03 |
| ATOM | 6579 | H   | LYS | 202 | 22.380 | -26.224 | -16.139 | 1.00 | 0.00  |
| ATOM | 6580 | HZ1 | LYS | 202 | 21.851 | -32.701 | -15.208 | 1.00 | 0.00  |
| ATOM | 6581 | HZ2 | LYS | 202 | 21.327 | -33.497 | -16.585 | 1.00 | 0.00  |
| ATOM | 6582 | HZ3 | LYS | 202 | 20.180 | -32.892 | -15.480 | 1.00 | 0.00  |
| ATOM | 6583 | N   | VAL | 203 | 25.507 | -28.524 | -15.502 | 1.00 | 46.37 |
| ATOM | 6584 | CA  | VAL | 203 | 26.927 | -28.619 | -15.826 | 1.00 | 48.08 |
| ATOM | 6585 | C   | VAL | 203 | 27.372 | -30.065 | -15.900 | 1.00 | 49.20 |
| ATOM | 6586 | O   | VAL | 203 | 27.544 | -30.730 | -14.877 | 1.00 | 48.26 |
| ATOM | 6587 | CB  | VAL | 203 | 27.801 | -27.881 | -14.800 | 1.00 | 48.34 |
| ATOM | 6588 | CG1 | VAL | 203 | 29.279 | -28.070 | -15.136 | 1.00 | 48.37 |
| ATOM | 6589 | CG2 | VAL | 203 | 27.444 | -26.405 | -14.782 | 1.00 | 48.31 |
| ATOM | 6590 | H   | VAL | 203 | 25.234 | -28.693 | -14.573 | 1.00 | 0.00  |
| ATOM | 6591 | N   | ASN | 204 | 27.569 | -30.533 | -17.128 | 1.00 | 51.36 |
| ATOM | 6592 | CA  | ASN | 204 | 27.998 | -31.902 | -17.388 | 1.00 | 52.84 |
| ATOM | 6593 | C   | ASN | 204 | 27.224 | -32.891 | -16.530 | 1.00 | 52.15 |
| ATOM | 6594 | O   | ASN | 204 | 27.750 | -33.463 | -15.573 | 1.00 | 52.01 |
| ATOM | 6595 | CB  | ASN | 204 | 29.510 | -32.060 | -17.164 | 1.00 | 55.18 |

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|      |      |      |     |     |        |         |         |      |       |
|------|------|------|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6596 | CG   | ASN | 204 | 30.347 | -31.520 | -18.328 | 1.00 | 57.60 |
| ATOM | 6597 | OD1  | ASN | 204 | 31.575 | -31.569 | -18.287 | 1.00 | 59.24 |
| ATOM | 6598 | ND2  | ASN | 204 | 29.687 | -31.015 | -19.371 | 1.00 | 58.19 |
| ATOM | 6599 | H    | ASN | 204 | 27.393 | -29.907 | -17.860 | 1.00 | 0.00  |
| ATOM | 6600 | HD21 | ASN | 204 | 28.718 | -30.974 | -19.440 | 1.00 | 0.00  |
| ATOM | 6601 | HD22 | ASN | 204 | 30.289 | -30.695 | -20.076 | 1.00 | 0.00  |
| ATOM | 6602 | N    | GLY | 205 | 25.957 | -33.075 | -16.875 | 1.00 | 51.28 |
| ATOM | 6603 | CA   | GLY | 205 | 25.133 | -33.994 | -16.123 | 1.00 | 50.61 |
| ATOM | 6604 | C    | GLY | 205 | 24.649 | -33.371 | -14.830 | 1.00 | 50.05 |
| ATOM | 6605 | O    | GLY | 205 | 23.497 | -32.937 | -14.751 | 1.00 | 52.30 |
| ATOM | 6606 | H    | GLY | 205 | 25.587 | -32.580 | -17.629 | 1.00 | 0.00  |
| ATOM | 6607 | N    | THR | 206 | 25.528 | -33.274 | -13.839 | 1.00 | 47.21 |
| ATOM | 6608 | CA   | THR | 206 | 25.168 | -32.719 | -12.537 | 1.00 | 43.80 |
| ATOM | 6609 | C    | THR | 206 | 24.671 | -31.275 | -12.508 | 1.00 | 40.99 |
| ATOM | 6610 | O    | THR | 206 | 25.148 | -30.419 | -13.256 | 1.00 | 40.64 |
| ATOM | 6611 | CB   | THR | 206 | 26.320 | -32.887 | -11.524 | 1.00 | 44.25 |
| ATOM | 6612 | OG1  | THR | 206 | 27.563 | -33.055 | -12.223 | 1.00 | 45.62 |
| ATOM | 6613 | CG2  | THR | 206 | 26.070 | -34.102 | -10.644 | 1.00 | 44.19 |
| ATOM | 6614 | H    | THR | 206 | 26.456 | -33.569 | -13.982 | 1.00 | 0.00  |
| ATOM | 6615 | HG1  | THR | 206 | 27.666 | -32.360 | -12.896 | 1.00 | 0.00  |
| ATOM | 6616 | N    | TRP | 207 | 23.649 | -31.044 | -11.690 | 1.00 | 38.59 |
| ATOM | 6617 | CA   | TRP | 207 | 23.073 | -29.720 | -11.515 | 1.00 | 36.46 |
| ATOM | 6618 | C    | TRP | 207 | 23.920 | -29.070 | -10.442 | 1.00 | 34.43 |
| ATOM | 6619 | O    | TRP | 207 | 24.178 | -29.680 | -9.404  | 1.00 | 35.65 |
| ATOM | 6620 | CB   | TRP | 207 | 21.629 | -29.796 | -10.992 | 1.00 | 37.90 |
| ATOM | 6621 | CG   | TRP | 207 | 20.563 | -29.997 | -12.031 | 1.00 | 39.17 |
| ATOM | 6622 | CD1  | TRP | 207 | 19.836 | -31.128 | -12.239 | 1.00 | 40.06 |
| ATOM | 6623 | CD2  | TRP | 207 | 20.096 | -29.039 | -12.995 | 1.00 | 39.34 |
| ATOM | 6624 | NE1  | TRP | 207 | 18.947 | -30.941 | -13.272 | 1.00 | 40.33 |
| ATOM | 6625 | CE2  | TRP | 207 | 19.085 | -29.669 | -13.756 | 1.00 | 39.24 |
| ATOM | 6626 | CE3  | TRP | 207 | 20.432 | -27.713 | -13.293 | 1.00 | 39.51 |
| ATOM | 6627 | CZ2  | TRP | 207 | 18.409 | -29.021 | -14.796 | 1.00 | 38.76 |
| ATOM | 6628 | CZ3  | TRP | 207 | 19.756 | -27.067 | -14.330 | 1.00 | 39.46 |
| ATOM | 6629 | CH2  | TRP | 207 | 18.757 | -27.725 | -15.067 | 1.00 | 38.53 |
| ATOM | 6630 | H    | TRP | 207 | 23.311 | -31.768 | -11.133 | 1.00 | 0.00  |
| ATOM | 6631 | HE1  | TRP | 207 | 18.288 | -31.604 | -13.566 | 1.00 | 0.00  |
| ATOM | 6632 | N    | LEU | 208 | 24.361 | -27.845 | -10.683 | 1.00 | 30.99 |
| ATOM | 6633 | CA   | LEU | 208 | 25.158 | -27.140 | -9.697  | 1.00 | 28.84 |
| ATOM | 6634 | C    | LEU | 208 | 24.458 | -25.835 | -9.330  | 1.00 | 28.19 |
| ATOM | 6635 | O    | LEU | 208 | 23.900 | -25.162 | -10.203 | 1.00 | 29.30 |
| ATOM | 6636 | CB   | LEU | 208 | 26.541 | -26.845 | -10.263 | 1.00 | 28.96 |
| ATOM | 6637 | CG   | LEU | 208 | 27.318 | -28.014 | -10.861 | 1.00 | 29.11 |
| ATOM | 6638 | CD1  | LEU | 208 | 28.641 | -27.486 | -11.393 | 1.00 | 30.26 |
| ATOM | 6639 | CD2  | LEU | 208 | 27.549 | -29.103 | -9.822  | 1.00 | 28.70 |
| ATOM | 6640 | H    | LEU | 208 | 24.159 | -27.435 | -11.550 | 1.00 | 0.00  |
| ATOM | 6641 | N    | GLN | 209 | 24.432 | -25.496 | -8.043  | 1.00 | 26.54 |
| ATOM | 6642 | CA   | GLN | 209 | 23.795 | -24.250 | -7.633  | 1.00 | 25.71 |
| ATOM | 6643 | C    | GLN | 209 | 24.765 | -23.107 | -7.856  | 1.00 | 24.56 |
| ATOM | 6644 | O    | GLN | 209 | 25.604 | -22.815 | -7.002  | 1.00 | 24.28 |
| ATOM | 6645 | CB   | GLN | 209 | 23.331 | -24.270 | -6.171  | 1.00 | 26.24 |
| ATOM | 6646 | CG   | GLN | 209 | 22.574 | -22.988 | -5.777  | 1.00 | 26.14 |
| ATOM | 6647 | CD   | GLN | 209 | 21.934 | -23.034 | -4.395  | 1.00 | 26.48 |
| ATOM | 6648 | OE1  | GLN | 209 | 21.284 | -22.077 | -3.977  | 1.00 | 27.75 |
| ATOM | 6649 | NE2  | GLN | 209 | 22.111 | -24.137 | -3.684  | 1.00 | 26.12 |
| ATOM | 6650 | H    | GLN | 209 | 24.840 | -26.121 | -7.400  | 1.00 | 0.00  |
| ATOM | 6651 | HE21 | GLN | 209 | 22.655 | -24.897 | -3.954  | 1.00 | 0.00  |
| ATOM | 6652 | HE22 | GLN | 209 | 21.587 | -24.089 | -2.856  | 1.00 | 0.00  |
| ATOM | 6653 | N    | ALA | 210 | 24.625 | -22.462 | -9.009  | 1.00 | 23.35 |
| ATOM | 6654 | CA   | ALA | 210 | 25.478 | -21.348 | -9.397  | 1.00 | 22.24 |
| ATOM | 6655 | C    | ALA | 210 | 25.290 | -20.130 | -8.514  | 1.00 | 21.09 |
| ATOM | 6656 | O    | ALA | 210 | 26.261 | -19.557 | -8.004  | 1.00 | 21.42 |
| ATOM | 6657 | CB   | ALA | 210 | 25.225 | -20.982 | -10.841 | 1.00 | 22.75 |
| ATOM | 6658 | H    | ALA | 210 | 23.892 | -22.733 | -9.603  | 1.00 | 0.00  |

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|      |      |     |     |     |        |         |         |      |       |
|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6659 | N   | GLY | 211 | 24.040 | -19.741 | -8.316  | 1.00 | 19.37 |
| ATOM | 6660 | CA  | GLY | 211 | 23.795 | -18.577 | -7.502  | 1.00 | 17.64 |
| ATOM | 6661 | C   | GLY | 211 | 22.568 | -18.677 | -6.644  | 1.00 | 16.46 |
| ATOM | 6662 | O   | GLY | 211 | 21.914 | -19.725 | -6.578  | 1.00 | 14.97 |
| ATOM | 6663 | H   | GLY | 211 | 23.301 | -20.270 | -8.679  | 1.00 | 0.00  |
| ATOM | 6664 | N   | VAL | 212 | 22.254 | -17.547 | -6.022  | 1.00 | 16.39 |
| ATOM | 6665 | CA  | VAL | 212 | 21.111 | -17.390 | -5.129  | 1.00 | 16.42 |
| ATOM | 6666 | C   | VAL | 212 | 20.413 | -16.088 | -5.555  | 1.00 | 17.78 |
| ATOM | 6667 | O   | VAL | 212 | 21.088 | -15.105 | -5.856  | 1.00 | 21.70 |
| ATOM | 6668 | CB  | VAL | 212 | 21.601 | -17.257 | -3.666  | 1.00 | 14.63 |
| ATOM | 6669 | CG1 | VAL | 212 | 20.435 | -17.100 | -2.726  | 1.00 | 16.34 |
| ATOM | 6670 | CG2 | VAL | 212 | 22.436 | -18.463 | -3.276  | 1.00 | 13.21 |
| ATOM | 6671 | H   | VAL | 212 | 22.823 | -16.764 | -6.174  | 1.00 | 0.00  |
| ATOM | 6672 | N   | VAL | 213 | 19.082 | -16.083 | -5.615  | 1.00 | 15.90 |
| ATOM | 6673 | CA  | VAL | 213 | 18.325 | -14.891 | -6.018  | 1.00 | 15.13 |
| ATOM | 6674 | C   | VAL | 213 | 18.503 | -13.786 | -4.986  | 1.00 | 18.46 |
| ATOM | 6675 | O   | VAL | 213 | 17.893 | -13.838 | -3.912  | 1.00 | 20.95 |
| ATOM | 6676 | CB  | VAL | 213 | 16.833 | -15.188 | -6.141  | 1.00 | 12.87 |
| ATOM | 6677 | CG1 | VAL | 213 | 16.130 | -14.013 | -6.751  | 1.00 | 11.61 |
| ATOM | 6678 | CG2 | VAL | 213 | 16.609 | -16.418 | -6.975  | 1.00 | 13.44 |
| ATOM | 6679 | H   | VAL | 213 | 18.628 | -16.914 | -5.381  | 1.00 | 0.00  |
| ATOM | 6680 | N   | SER | 214 | 19.286 | -12.768 | -5.335  | 1.00 | 20.04 |
| ATOM | 6681 | CA  | SER | 214 | 19.586 | -11.668 | -4.421  | 1.00 | 21.15 |
| ATOM | 6682 | C   | SER | 214 | 18.839 | -10.348 | -4.641  | 1.00 | 21.80 |
| ATOM | 6683 | O   | SER | 214 | 18.095 | -9.913  | -3.765  | 1.00 | 22.00 |
| ATOM | 6684 | CB  | SER | 214 | 21.102 | -11.426 | -4.412  | 1.00 | 22.01 |
| ATOM | 6685 | OG  | SER | 214 | 21.474 | -10.349 | -3.572  | 1.00 | 22.72 |
| ATOM | 6686 | H   | SER | 214 | 19.678 | -12.718 | -6.237  | 1.00 | 0.00  |
| ATOM | 6687 | HG  | SER | 214 | 21.364 | -10.653 | -2.664  | 1.00 | 0.00  |
| ATOM | 6688 | N   | TRP | 215 | 19.067 | -9.687  | -5.774  | 1.00 | 23.44 |
| ATOM | 6689 | CA  | TRP | 215 | 18.407 | -8.410  | -6.044  | 1.00 | 25.65 |
| ATOM | 6690 | C   | TRP | 215 | 18.229 | -8.096  | -7.527  | 1.00 | 26.77 |
| ATOM | 6691 | O   | TRP | 215 | 18.471 | -8.946  | -8.387  | 1.00 | 25.97 |
| ATOM | 6692 | CB  | TRP | 215 | 19.134 | -7.245  | -5.335  | 1.00 | 27.15 |
| ATOM | 6693 | CG  | TRP | 215 | 20.481 | -6.825  | -5.917  | 1.00 | 28.74 |
| ATOM | 6694 | CD1 | TRP | 215 | 21.649 | -7.518  | -5.847  | 1.00 | 29.32 |
| ATOM | 6695 | CD2 | TRP | 215 | 20.784 | -5.604  | -6.626  | 1.00 | 29.57 |
| ATOM | 6696 | NE1 | TRP | 215 | 22.656 | -6.816  | -6.461  | 1.00 | 29.92 |
| ATOM | 6697 | CE2 | TRP | 215 | 22.156 | -5.640  | -6.951  | 1.00 | 28.88 |
| ATOM | 6698 | CE3 | TRP | 215 | 20.027 | -4.487  | -7.015  | 1.00 | 31.43 |
| ATOM | 6699 | CZ2 | TRP | 215 | 22.794 | -4.607  | -7.651  | 1.00 | 29.19 |
| ATOM | 6700 | CZ3 | TRP | 215 | 20.665 | -3.453  | -7.714  | 1.00 | 30.67 |
| ATOM | 6701 | CH2 | TRP | 215 | 22.037 | -3.527  | -8.022  | 1.00 | 28.91 |
| ATOM | 6702 | H   | TRP | 215 | 19.648 | -10.073 | -6.469  | 1.00 | 0.00  |
| ATOM | 6703 | HE1 | TRP | 215 | 23.586 | -7.127  | -6.519  | 1.00 | 0.00  |
| ATOM | 6704 | N   | GLY | 216 | 17.763 | -6.878  | -7.800  | 1.00 | 27.70 |
| ATOM | 6705 | CA  | GLY | 216 | 17.539 | -6.419  | -9.159  | 1.00 | 30.66 |
| ATOM | 6706 | C   | GLY | 216 | 16.542 | -5.275  | -9.124  | 1.00 | 33.49 |
| ATOM | 6707 | O   | GLY | 216 | 15.815 | -5.137  | -8.142  | 1.00 | 35.70 |
| ATOM | 6708 | H   | GLY | 216 | 17.526 | -6.262  | -7.076  | 1.00 | 0.00  |
| ATOM | 6709 | N   | GLU | 217 | 16.531 | -4.431  | -10.153 | 1.00 | 34.80 |
| ATOM | 6710 | CA  | GLU | 217 | 15.595 | -3.302  | -10.221 | 1.00 | 35.38 |
| ATOM | 6711 | C   | GLU | 217 | 14.288 | -3.733  | -10.901 | 1.00 | 34.97 |
| ATOM | 6712 | O   | GLU | 217 | 14.105 | -3.545  | -12.104 | 1.00 | 36.03 |
| ATOM | 6713 | CB  | GLU | 217 | 16.223 | -2.103  | -10.966 | 1.00 | 37.29 |
| ATOM | 6714 | CG  | GLU | 217 | 17.397 | -1.421  | -10.224 | 1.00 | 39.90 |
| ATOM | 6715 | CD  | GLU | 217 | 17.968 | -0.196  | -10.947 | 1.00 | 39.47 |
| ATOM | 6716 | OE1 | GLU | 217 | 19.122 | -0.260  | -11.417 | 1.00 | 39.59 |
| ATOM | 6717 | OE2 | GLU | 217 | 17.278 | 0.838   | -11.031 | 1.00 | 39.08 |
| ATOM | 6718 | H   | GLU | 217 | 17.179 | -4.583  | -10.877 | 1.00 | 0.00  |
| ATOM | 6719 | N   | GLY | 219 | 13.371 | -4.296  | -10.126 | 1.00 | 33.56 |
| ATOM | 6720 | CA  | GLY | 219 | 12.116 | -4.746  | -10.691 | 1.00 | 32.04 |
| ATOM | 6721 | C   | GLY | 219 | 12.249 | -6.189  | -11.122 | 1.00 | 31.59 |

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|      |      |      |     |      |        |        |         |      |       |
|------|------|------|-----|------|--------|--------|---------|------|-------|
| ATOM | 6722 | O    | GLY | 219  | 13.151 | -6.887 | -10.659 | 1.00 | 31.71 |
| ATOM | 6723 | H    | GLY | 219  | 13.527 | -4.434 | -9.166  | 1.00 | 0.00  |
| ATOM | 6724 | N    | CYS | 220  | 11.336 | -6.642 | -11.977 | 1.00 | 31.16 |
| ATOM | 6725 | CA   | CYS | 220  | 11.347 | -8.012 | -12.482 | 1.00 | 29.45 |
| ATOM | 6726 | C    | CYS | 220  | 11.210 | -8.000 | -14.001 | 1.00 | 29.22 |
| ATOM | 6727 | O    | CYS | 220  | 10.277 | -7.407 | -14.540 | 1.00 | 29.78 |
| ATOM | 6728 | CB   | CYS | 220  | 10.191 | -8.800 | -11.879 | 1.00 | 26.84 |
| ATOM | 6729 | SG   | CYS | 220  | 10.118 | -8.745 | -10.067 | 1.00 | 24.11 |
| ATOM | 6730 | H    | CYS | 220  | 10.601 | -6.083 | -12.299 | 1.00 | 0.00  |
| ATOM | 6731 | N    | ALA | 221  | 12.152 | -8.641 | -14.685 | 1.00 | 28.48 |
| ATOM | 6732 | CA   | ALA | 221  | 12.162 | -8.703 | -16.142 | 1.00 | 28.12 |
| ATOM | 6733 | C    | ALA | 221  | 12.144 | -7.304 | -16.760 | 1.00 | 28.63 |
| ATOM | 6734 | O    | ALA | 221  | 11.514 | -7.086 | -17.791 | 1.00 | 28.69 |
| ATOM | 6735 | CB   | ALA | 221  | 10.985 | -9.528 | -16.648 | 1.00 | 26.67 |
| ATOM | 6736 | H    | ALA | 221  | 12.861 | -9.086 | -14.179 | 1.00 | 0.00  |
| ATOM | 6737 | N    | GLN | 221A | 12.863 | -6.372 | -16.140 | 1.00 | 29.21 |
| ATOM | 6738 | CA   | GLN | 221A | 12.947 | -4.983 | -16.610 | 1.00 | 29.30 |
| ATOM | 6739 | C    | GLN | 221A | 14.060 | -4.782 | -17.643 | 1.00 | 28.92 |
| ATOM | 6740 | O    | GLN | 221A | 15.148 | -5.355 | -17.515 | 1.00 | 29.52 |
| ATOM | 6741 | CB   | GLN | 221A | 13.188 | -4.038 | -15.429 | 1.00 | 30.02 |
| ATOM | 6742 | CG   | GLN | 221A | 12.007 | -3.876 | -14.489 | 1.00 | 31.52 |
| ATOM | 6743 | CD   | GLN | 221A | 10.976 | -2.503 | -15.012 | 1.00 | 32.45 |
| ATOM | 6744 | OE1  | GLN | 221A | 9.842  | -3.275 | -15.306 | 1.00 | 33.26 |
| ATOM | 6745 | NE2  | GLN | 221A | 11.363 | -1.640 | -15.116 | 1.00 | 33.17 |
| ATOM | 6746 | H    | GLN | 221A | 13.404 | -6.645 | -15.367 | 1.00 | 0.00  |
| ATOM | 6747 | HE21 | GLN | 221A | 12.278 | -1.411 | -14.849 | 1.00 | 0.00  |
| ATOM | 6748 | HE22 | GLN | 221A | 10.703 | -1.008 | -15.461 | 1.00 | 0.00  |
| ATOM | 6749 | N    | PRO | 222  | 13.810 | -3.948 | -18.674 | 1.00 | 28.32 |
| ATOM | 6750 | CA   | PRO | 222  | 14.795 | -3.669 | -19.729 | 1.00 | 27.33 |
| ATOM | 6751 | C    | PRO | 222  | 16.116 | -3.136 | -19.162 | 1.00 | 27.39 |
| ATOM | 6752 | O    | PRO | 222  | 16.125 | -2.226 | -18.324 | 1.00 | 28.99 |
| ATOM | 6753 | CB   | PRO | 222  | 14.093 | -2.609 | -20.580 | 1.00 | 26.61 |
| ATOM | 6754 | CG   | PRO | 222  | 12.645 | -2.930 | -20.400 | 1.00 | 26.93 |
| ATOM | 6755 | CD   | PRO | 222  | 12.557 | -3.209 | -18.923 | 1.00 | 27.93 |
| ATOM | 6756 | N    | ASN | 223  | 17.223 | -3.725 | -19.612 | 1.00 | 25.39 |
| ATOM | 6757 | CA   | ASN | 223  | 18.565 | -3.346 | -19.175 | 1.00 | 22.48 |
| ATOM | 6758 | C    | ASN | 223  | 18.787 | -3.547 | -17.682 | 1.00 | 21.50 |
| ATOM | 6759 | O    | ASN | 223  | 19.623 | -2.869 | -17.087 | 1.00 | 22.68 |
| ATOM | 6760 | CB   | ASN | 223  | 18.869 | -1.895 | -19.548 | 1.00 | 21.76 |
| ATOM | 6761 | CG   | ASN | 223  | 18.848 | -1.662 | -21.036 | 1.00 | 22.23 |
| ATOM | 6762 | OD1  | ASN | 223  | 18.353 | -0.642 | -21.511 | 1.00 | 24.31 |
| ATOM | 6763 | ND2  | ASN | 223  | 19.391 | -2.607 | -21.787 | 1.00 | 23.45 |
| ATOM | 6764 | H    | ASN | 223  | 17.103 | -4.445 | -20.258 | 1.00 | 0.00  |
| ATOM | 6765 | HD21 | ASN | 223  | 19.786 | -3.395 | -21.380 | 1.00 | 0.00  |
| ATOM | 6766 | HD22 | ASN | 223  | 19.368 | -2.423 | -22.748 | 1.00 | 0.00  |
| ATOM | 6767 | N    | ARG | 224  | 18.024 | -4.453 | -17.078 | 1.00 | 19.10 |
| ATOM | 6768 | CA   | ARG | 224  | 18.145 | -4.746 | -15.653 | 1.00 | 18.27 |
| ATOM | 6769 | C    | ARG | 224  | 17.947 | -6.246 | -15.360 | 1.00 | 19.54 |
| ATOM | 6770 | O    | ARG | 224  | 16.875 | -6.678 | -14.909 | 1.00 | 19.90 |
| ATOM | 6771 | CB   | ARG | 224  | 17.121 | -3.938 | -14.863 | 1.00 | 16.15 |
| ATOM | 6772 | CG   | ARG | 224  | 17.224 | -2.448 | -15.019 | 1.00 | 15.73 |
| ATOM | 6773 | CD   | ARG | 224  | 18.406 | -1.911 | -14.259 | 1.00 | 16.61 |
| ATOM | 6774 | NE   | ARG | 224  | 18.401 | -0.448 | -14.180 | 1.00 | 16.66 |
| ATOM | 6775 | CZ   | ARG | 224  | 18.801 | 0.363  | -15.156 | 1.00 | 14.80 |
| ATOM | 6776 | NH1  | ARG | 224  | 19.235 | -0.142 | -16.307 | 1.00 | 12.82 |
| ATOM | 6777 | NH2  | ARG | 224  | 18.819 | 1.677  | -14.959 | 1.00 | 13.81 |
| ATOM | 6778 | H    | ARG | 224  | 17.290 | -4.913 | -17.540 | 1.00 | 0.00  |
| ATOM | 6779 | HE   | ARG | 224  | 18.108 | -0.049 | -13.316 | 1.00 | 0.00  |
| ATOM | 6780 | HH11 | ARG | 224  | 19.309 | -1.130 | -16.488 | 1.00 | 0.00  |
| ATOM | 6781 | HH12 | ARG | 224  | 19.558 | 0.486  | -17.016 | 1.00 | 0.00  |
| ATOM | 6782 | HH21 | ARG | 224  | 18.512 | 2.079  | -14.068 | 1.00 | 0.00  |
| ATOM | 6783 | HH22 | ARG | 224  | 19.132 | 2.309  | -15.661 | 1.00 | 0.00  |
| ATOM | 6784 | N    | PRO | 225  | 18.944 | -7.077 | -15.706 | 1.00 | 18.61 |

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|      |      |      |     |     |        |         |         |      |       |
|------|------|------|-----|-----|--------|---------|---------|------|-------|
| ATOM | 6785 | CA   | PRO | 225 | 18.818 | -8.511  | -15.446 | 1.00 | 17.77 |
| ATOM | 6786 | C    | PRO | 225 | 18.833 | -8.753  | -13.939 | 1.00 | 18.57 |
| ATOM | 6787 | O    | PRO | 225 | 19.244 | -7.874  | -13.174 | 1.00 | 19.67 |
| ATOM | 6788 | CB   | PRO | 225 | 20.067 | -9.074  | -16.110 | 1.00 | 16.82 |
| ATOM | 6789 | CG   | PRO | 225 | 20.269 | -8.147  | -17.253 | 1.00 | 16.81 |
| ATOM | 6790 | CD   | PRO | 225 | 20.096 | -6.818  | -16.581 | 1.00 | 18.08 |
| ATOM | 6791 | N    | GLY | 226 | 18.360 | -9.919  | -13.513 | 1.00 | 18.16 |
| ATOM | 6792 | CA   | GLY | 226 | 18.340 | -10.230 | -12.097 | 1.00 | 17.73 |
| ATOM | 6793 | C    | GLY | 226 | 19.736 | -10.516 | -11.595 | 1.00 | 17.93 |
| ATOM | 6794 | O    | GLY | 226 | 20.527 | -11.149 | -12.288 | 1.00 | 19.71 |
| ATOM | 6795 | H    | GLY | 226 | 17.996 | -10.604 | -14.113 | 1.00 | 0.00  |
| ATOM | 6796 | N    | ILE | 227 | 20.069 | -10.021 | -10.414 | 1.00 | 17.86 |
| ATOM | 6797 | CA   | ILE | 227 | 21.387 | -10.273 | -9.857  | 1.00 | 18.04 |
| ATOM | 6798 | C    | ILE | 227 | 21.294 | -11.391 | -8.820  | 1.00 | 18.05 |
| ATOM | 6799 | O    | ILE | 227 | 20.384 | -11.419 | -7.984  | 1.00 | 19.22 |
| ATOM | 6800 | CB   | ILE | 227 | 22.007 | -9.006  | -9.229  | 1.00 | 17.62 |
| ATOM | 6801 | CG1  | ILE | 227 | 22.409 | -8.017  | -10.315 | 1.00 | 17.91 |
| ATOM | 6802 | CG2  | ILE | 227 | 23.254 | -9.357  | -8.460  | 1.00 | 19.38 |
| ATOM | 6803 | H    | ILE | 227 | 19.422 | -9.521  | -9.884  | 1.00 | 0.00  |
| ATOM | 6804 | CD   | ILE | 227 | 21.261 | -7.439  | -11.054 | 1.00 | 18.79 |
| ATOM | 6805 | N    | TYR | 228 | 22.216 | -12.334 | -8.912  | 1.00 | 15.79 |
| ATOM | 6806 | CA   | TYR | 228 | 22.259 | -13.460 | -8.003  | 1.00 | 16.65 |
| ATOM | 6807 | C    | TYR | 228 | 23.587 | -13.430 | -7.257  | 1.00 | 17.80 |
| ATOM | 6808 | O    | TYR | 228 | 24.552 | -12.831 | -7.728  | 1.00 | 19.28 |
| ATOM | 6809 | CB   | TYR | 228 | 22.153 | -14.769 | -8.795  | 1.00 | 16.56 |
| ATOM | 6810 | CG   | TYR | 228 | 20.902 | -14.884 | -9.634  | 1.00 | 17.28 |
| ATOM | 6811 | CD1  | TYR | 228 | 20.721 | -14.092 | -10.766 | 1.00 | 17.78 |
| ATOM | 6812 | CD2  | TYR | 228 | 19.873 | -15.754 | -9.274  | 1.00 | 16.86 |
| ATOM | 6813 | CE1  | TYR | 228 | 19.542 | -14.157 | -11.509 | 1.00 | 16.84 |
| ATOM | 6814 | CE2  | TYR | 228 | 18.694 | -15.823 | -10.013 | 1.00 | 14.56 |
| ATOM | 6815 | CZ   | TYR | 228 | 18.538 | -15.020 | -11.120 | 1.00 | 15.15 |
| ATOM | 6816 | OH   | TYR | 228 | 17.359 | -15.039 | -11.814 | 1.00 | 16.78 |
| ATOM | 6817 | H    | TYR | 228 | 22.875 | -12.262 | -9.601  | 1.00 | 0.00  |
| ATOM | 6818 | HH   | TYR | 228 | 16.641 | -14.838 | -11.203 | 1.00 | 0.00  |
| ATOM | 6819 | N    | THR | 229 | 23.639 | -14.048 | -6.085  | 1.00 | 16.85 |
| ATOM | 6820 | CA   | THR | 229 | 24.885 | -14.097 | -5.340  | 1.00 | 17.23 |
| ATOM | 6821 | C    | THR | 229 | 25.679 | -15.207 | -5.995  | 1.00 | 18.33 |
| ATOM | 6822 | O    | THR | 229 | 25.112 | -16.240 | -6.355  | 1.00 | 19.18 |
| ATOM | 6823 | CB   | THR | 229 | 24.659 | -14.483 | -3.879  | 1.00 | 16.41 |
| ATOM | 6824 | OG1  | THR | 229 | 23.586 | -13.705 | -3.347  | 1.00 | 18.40 |
| ATOM | 6825 | CG2  | THR | 229 | 25.913 | -14.216 | -3.065  | 1.00 | 16.08 |
| ATOM | 6826 | H    | THR | 229 | 22.835 | -14.458 | -5.726  | 1.00 | 0.00  |
| ATOM | 6827 | HG1  | THR | 229 | 23.919 | -12.996 | -2.782  | 1.00 | 0.00  |
| ATOM | 6828 | N    | ARG | 230 | 26.968 | -14.982 | -6.198  | 1.00 | 18.45 |
| ATOM | 6829 | CA   | ARG | 230 | 27.806 | -15.992 | -6.811  | 1.00 | 21.08 |
| ATOM | 6830 | C    | ARG | 230 | 28.263 | -16.954 | -5.725  | 1.00 | 24.17 |
| ATOM | 6831 | O    | ARG | 230 | 29.024 | -16.577 | -4.834  | 1.00 | 25.89 |
| ATOM | 6832 | CB   | ARG | 230 | 28.995 | -15.338 | -7.512  | 1.00 | 22.59 |
| ATOM | 6833 | CG   | ARG | 230 | 30.109 | -16.297 | -7.888  | 1.00 | 24.75 |
| ATOM | 6834 | CD   | ARG | 230 | 31.067 | -15.680 | -8.883  | 1.00 | 25.61 |
| ATOM | 6835 | NE   | ARG | 230 | 30.665 | -15.951 | -10.260 | 1.00 | 26.94 |
| ATOM | 6836 | CZ   | ARG | 230 | 30.154 | -15.040 | -11.080 | 1.00 | 27.48 |
| ATOM | 6837 | NH1  | ARG | 230 | 29.978 | -13.800 | -10.647 | 1.00 | 28.61 |
| ATOM | 6838 | NH2  | ARG | 230 | 29.867 | -15.354 | -12.342 | 1.00 | 26.98 |
| ATOM | 6839 | H    | ARG | 230 | 27.357 | -14.134 | -5.903  | 1.00 | 0.00  |
| ATOM | 6840 | HE   | ARG | 230 | 30.801 | -16.890 | -10.525 | 1.00 | 0.00  |
| ATOM | 6841 | HH11 | ARG | 230 | 30.249 | -13.518 | -9.722  | 1.00 | 0.00  |
| ATOM | 6842 | HH12 | ARG | 230 | 29.589 | -13.050 | -11.204 | 1.00 | 0.00  |
| ATOM | 6843 | HH21 | ARG | 230 | 30.021 | -16.266 | -12.719 | 1.00 | 0.00  |
| ATOM | 6844 | HH22 | ARG | 230 | 29.490 | -14.661 | -12.970 | 1.00 | 0.00  |
| ATOM | 6845 | N    | VAL | 231 | 27.806 | -18.203 | -5.806  | 1.00 | 26.09 |
| ATOM | 6846 | CA   | VAL | 231 | 28.153 | -19.205 | -4.804  | 1.00 | 26.32 |
| ATOM | 6847 | C    | VAL | 231 | 29.636 | -19.546 | -4.730  | 1.00 | 26.68 |

|      |      |     |     |     |         |         |         |      |       |
|------|------|-----|-----|-----|---------|---------|---------|------|-------|
| ATOM | 9305 | CE1 | TYR | 241 | -37.718 | -19.089 | -12.144 | 1.00 | 33.56 |
| ATOM | 9306 | CE2 | TYR | 241 | -37.143 | -19.342 | -14.462 | 1.00 | 32.65 |
| ATOM | 9307 | CZ  | TYR | 241 | -37.644 | -18.574 | -13.427 | 1.00 | 33.47 |
| ATOM | 9308 | OH  | TYR | 241 | -38.081 | -17.297 | -13.681 | 1.00 | 34.49 |
| ATOM | 9309 | H   | TYR | 241 | -38.465 | -23.017 | -11.046 | 1.00 | 0.00  |
| ATOM | 9310 | HH  | TYR | 241 | -38.272 | -16.853 | -12.855 | 1.00 | 0.00  |
| ATOM | 9311 | N   | VAL | 242 | -36.881 | -25.165 | -11.086 | 1.00 | 36.66 |
| ATOM | 9312 | CA  | VAL | 242 | -36.417 | -26.435 | -10.548 | 1.00 | 37.99 |
| ATOM | 9313 | C   | VAL | 242 | -37.625 | -27.328 | -10.253 | 1.00 | 41.56 |
| ATOM | 9314 | O   | VAL | 242 | -38.377 | -27.078 | -9.301  | 1.00 | 41.79 |
| ATOM | 9315 | CB  | VAL | 242 | -35.585 | -26.210 | -9.280  | 1.00 | 37.17 |
| ATOM | 9316 | CG1 | VAL | 242 | -34.923 | -27.500 | -8.848  | 1.00 | 36.94 |
| ATOM | 9317 | CG2 | VAL | 242 | -34.543 | -25.135 | -9.531  | 1.00 | 36.67 |
| ATOM | 9318 | H   | VAL | 242 | -37.122 | -24.457 | -10.468 | 1.00 | 0.00  |
| ATOM | 9319 | N   | PRO | 243 | -37.793 | -28.408 | -11.040 | 1.00 | 43.68 |
| ATOM | 9320 | CA  | PRO | 243 | -38.879 | -29.386 | -10.945 | 1.00 | 46.84 |
| ATOM | 9321 | C   | PRO | 243 | -39.004 | -30.118 | -9.625  | 1.00 | 50.05 |
| ATOM | 9322 | O   | PRO | 243 | -38.102 | -30.092 | -8.788  | 1.00 | 49.11 |
| ATOM | 9323 | CB  | PRO | 243 | -38.551 | -30.364 | -12.072 | 1.00 | 45.09 |
| ATOM | 9324 | CG  | PRO | 243 | -37.075 | -30.359 | -12.074 | 1.00 | 44.34 |
| ATOM | 9325 | CD  | PRO | 243 | -36.782 | -28.878 | -12.003 | 1.00 | 44.28 |
| ATOM | 9326 | N   | LYS | 244 | -40.143 | -30.783 | -9.464  | 1.00 | 55.29 |
| ATOM | 9327 | CA  | LYS | 244 | -40.438 | -31.565 | -8.276  | 1.00 | 60.05 |
| ATOM | 9328 | C   | LYS | 244 | -39.625 | -32.860 | -8.352  | 1.00 | 63.67 |
| ATOM | 9329 | O   | LYS | 244 | -40.174 | -33.957 | -8.482  | 1.00 | 64.35 |
| ATOM | 9330 | CB  | LYS | 244 | -41.938 | -31.862 | -8.211  | 1.00 | 60.15 |
| ATOM | 9331 | CG  | LYS | 244 | -42.791 | -30.653 | -7.865  | 1.00 | 61.05 |
| ATOM | 9332 | CD  | LYS | 244 | -43.134 | -30.609 | -6.374  | 1.00 | 62.36 |
| ATOM | 9333 | CE  | LYS | 244 | -44.171 | -31.678 | -6.002  | 1.00 | 63.29 |
| ATOM | 9334 | NZ  | LYS | 244 | -44.659 | -31.607 | -4.580  | 1.00 | 64.30 |
| ATOM | 9335 | H   | LYS | 244 | -40.808 | -30.749 | -10.180 | 1.00 | 0.00  |
| ATOM | 9336 | HZ1 | LYS | 244 | -45.082 | -30.675 | -4.377  | 1.00 | 0.00  |
| ATOM | 9337 | HZ2 | LYS | 244 | -43.921 | -31.789 | -3.867  | 1.00 | 0.00  |
| ATOM | 9338 | HZ3 | LYS | 244 | -45.422 | -32.297 | -4.419  | 1.00 | 0.00  |
| ATOM | 9339 | N   | LYS | 245 | -38.305 | -32.705 | -8.309  | 1.00 | 66.44 |
| ATOM | 9340 | CA  | LYS | 245 | -37.373 | -33.820 | -8.370  | 1.00 | 68.53 |
| ATOM | 9341 | C   | LYS | 245 | -36.009 | -33.348 | -7.869  | 1.00 | 69.66 |
| ATOM | 9342 | O   | LYS | 245 | -35.294 | -32.619 | -8.566  | 1.00 | 70.41 |
| ATOM | 9343 | CB  | LYS | 245 | -37.240 | -34.342 | -9.803  | 1.00 | 69.23 |
| ATOM | 9344 | CG  | LYS | 245 | -36.186 | -35.419 | -9.942  | 1.00 | 70.70 |
| ATOM | 9345 | CD  | LYS | 245 | -35.327 | -35.202 | -11.173 | 1.00 | 72.47 |
| ATOM | 9346 | CE  | LYS | 245 | -34.068 | -36.061 | -11.112 | 1.00 | 74.04 |
| ATOM | 9347 | NZ  | LYS | 245 | -34.365 | -37.507 | -10.870 | 1.00 | 75.08 |
| ATOM | 9348 | H   | LYS | 245 | -37.914 | -31.819 | -8.196  | 1.00 | 0.00  |
| ATOM | 9349 | HZ1 | LYS | 245 | -35.012 | -37.891 | -11.588 | 1.00 | 0.00  |
| ATOM | 9350 | HZ2 | LYS | 245 | -34.836 | -37.655 | -9.955  | 1.00 | 0.00  |
| ATOM | 9351 | HZ3 | LYS | 245 | -33.480 | -38.050 | -10.886 | 1.00 | 0.00  |
| TER  | 9352 |     | LYS | 245 |         |         |         |      |       |
| ATOM | 9353 | C1  | APA | 301 | -23.052 | 9.766   | -6.085  | 1.00 | 21.89 |
| ATOM | 9354 | C2  | APA | 301 | -23.579 | 10.513  | -4.997  | 1.00 | 20.39 |
| ATOM | 9355 | C3  | APA | 301 | -23.246 | 10.302  | -3.667  | 1.00 | 19.04 |
| ATOM | 9356 | C4  | APA | 301 | -22.342 | 9.304   | -3.329  | 1.00 | 17.51 |
| ATOM | 9357 | C5  | APA | 301 | -21.830 | 8.581   | -4.399  | 1.00 | 18.86 |
| ATOM | 9358 | C6  | APA | 301 | -22.121 | 8.740   | -5.754  | 1.00 | 20.00 |
| ATOM | 9359 | C7  | APA | 301 | -23.466 | 10.066  | -7.399  | 1.00 | 23.77 |
| ATOM | 9360 | N8  | APA | 301 | -23.005 | 9.399   | -8.435  | 1.00 | 23.70 |
| ATOM | 9361 | N9  | APA | 301 | -24.338 | 11.024  | -7.665  | 1.00 | 25.12 |
| ATOM | 9362 | C10 | APA | 301 | -21.986 | 9.068   | -1.852  | 1.00 | 17.23 |
| ATOM | 9363 | O13 | APA | 301 | -21.090 | 11.219  | -1.509  | 1.00 | 17.21 |
| ATOM | 9364 | C13 | APA | 301 | -20.987 | 9.615   | 0.337   | 1.00 | 20.01 |
| ATOM | 9365 | O14 | APA | 301 | -19.653 | 9.921   | 0.187   | 1.00 | 22.87 |
| ATOM | 9366 | O15 | APA | 301 | -21.603 | 8.975   | 1.198   | 1.00 | 19.00 |
| ATOM | 9367 | C11 | APA | 301 | -21.854 | 10.224  | -0.842  | 1.00 | 17.64 |

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|         |      |     |     |     |         |         |         |      |       |
|---------|------|-----|-----|-----|---------|---------|---------|------|-------|
| TER     | 9368 |     | APA | 301 |         |         |         |      |       |
| ATOM    | 9369 | C1  | APA | 301 | 14.685  | 8.995   | 7.478   | 1.00 | 29.74 |
| ATOM    | 9370 | C2  | APA | 301 | 15.307  | 9.757   | 6.450   | 1.00 | 28.66 |
| ATOM    | 9371 | C3  | APA | 301 | 14.974  | 9.689   | 5.101   | 1.00 | 28.70 |
| ATOM    | 9372 | C4  | APA | 301 | 13.964  | 8.829   | 4.673   | 1.00 | 27.81 |
| ATOM    | 9373 | C5  | APA | 301 | 13.354  | 8.080   | 5.687   | 1.00 | 28.73 |
| ATOM    | 9374 | C6  | APA | 301 | 13.644  | 8.102   | 7.060   | 1.00 | 29.27 |
| ATOM    | 9375 | C7  | APA | 301 | 15.112  | 9.161   | 8.820   | 1.00 | 31.33 |
| ATOM    | 9376 | N8  | APA | 301 | 14.569  | 8.489   | 9.812   | 1.00 | 31.41 |
| ATOM    | 9377 | N9  | APA | 301 | 16.071  | 10.007  | 9.157   | 1.00 | 32.37 |
| ATOM    | 9378 | C10 | APA | 301 | 13.608  | 8.778   | 3.172   | 1.00 | 23.98 |
| ATOM    | 9379 | O13 | APA | 301 | 12.534  | 10.880  | 3.195   | 1.00 | 19.67 |
| ATOM    | 9380 | C13 | APA | 301 | 12.562  | 9.671   | 1.104   | 1.00 | 25.12 |
| ATOM    | 9381 | O14 | APA | 301 | 11.222  | 9.922   | 1.268   | 1.00 | 28.11 |
| ATOM    | 9382 | O15 | APA | 301 | 13.209  | 9.204   | 0.171   | 1.00 | 26.06 |
| ATOM    | 9383 | C11 | APA | 301 | 13.385  | 10.085  | 2.383   | 1.00 | 22.13 |
| TER     | 9384 |     | APA | 301 |         |         |         |      |       |
| ATOM    | 9385 | C1  | APA | 301 | 14.412  | -9.879  | -8.288  | 1.00 | 29.54 |
| ATOM    | 9386 | C2  | APA | 301 | 15.063  | -10.684 | -7.297  | 1.00 | 28.51 |
| ATOM    | 9387 | C3  | APA | 301 | 14.787  | -10.651 | -5.926  | 1.00 | 26.17 |
| ATOM    | 9388 | C4  | APA | 301 | 13.809  | -9.793  | -5.438  | 1.00 | 26.57 |
| ATOM    | 9389 | C5  | APA | 301 | 13.175  | -9.008  | -6.410  | 1.00 | 29.17 |
| ATOM    | 9390 | C6  | APA | 301 | 13.403  | -8.990  | -7.799  | 1.00 | 29.83 |
| ATOM    | 9391 | C7  | APA | 301 | 14.780  | -10.008 | -9.666  | 1.00 | 29.98 |
| ATOM    | 9392 | N8  | APA | 301 | 14.204  | -9.292  | -10.618 | 1.00 | 28.22 |
| ATOM    | 9393 | N9  | APA | 301 | 15.712  | -10.857 | -10.070 | 1.00 | 30.35 |
| ATOM    | 9394 | C10 | APA | 301 | 13.505  | -9.757  | -3.920  | 1.00 | 24.12 |
| ATOM    | 9395 | O13 | APA | 301 | 12.401  | -11.842 | -3.814  | 1.00 | 23.75 |
| ATOM    | 9396 | C13 | APA | 301 | 12.639  | -10.592 | -1.754  | 1.00 | 22.24 |
| ATOM    | 9397 | O14 | APA | 301 | 11.396  | -11.162 | -1.619  | 1.00 | 23.15 |
| ATOM    | 9398 | O15 | APA | 301 | 13.282  | -9.828  | -1.043  | 1.00 | 21.22 |
| ATOM    | 9399 | C11 | APA | 301 | 13.335  | -11.049 | -3.094  | 1.00 | 22.34 |
| TER     | 9400 |     | APA | 301 |         |         |         |      |       |
| ATOM    | 9401 | C1  | APA | 301 | -22.920 | -11.214 | 6.535   | 1.00 | 24.69 |
| ATOM    | 9402 | C2  | APA | 301 | -23.653 | -11.777 | 5.444   | 1.00 | 23.01 |
| ATOM    | 9403 | C3  | APA | 301 | -23.337 | -11.590 | 4.104   | 1.00 | 20.07 |
| ATOM    | 9404 | C4  | APA | 301 | -22.246 | -10.910 | 3.763   | 1.00 | 19.42 |
| ATOM    | 9405 | C5  | APA | 301 | -21.540 | -10.267 | 4.831   | 1.00 | 21.55 |
| ATOM    | 9406 | C6  | APA | 301 | -21.797 | -10.411 | 6.192   | 1.00 | 23.08 |
| ATOM    | 9407 | C7  | APA | 301 | -23.330 | -11.471 | 7.860   | 1.00 | 25.81 |
| ATOM    | 9408 | N8  | APA | 301 | -22.689 | -10.970 | 8.899   | 1.00 | 26.10 |
| ATOM    | 9409 | N9  | APA | 301 | -24.370 | -12.226 | 8.134   | 1.00 | 27.77 |
| ATOM    | 9410 | C10 | APA | 301 | -21.895 | -10.591 | 2.291   | 1.00 | 19.43 |
| ATOM    | 9411 | O13 | APA | 301 | -20.749 | -12.620 | 1.974   | 1.00 | 24.12 |
| ATOM    | 9412 | C13 | APA | 301 | -20.945 | -11.102 | 0.078   | 1.00 | 20.17 |
| ATOM    | 9413 | O14 | APA | 301 | -19.594 | -11.393 | 0.068   | 1.00 | 19.31 |
| ATOM    | 9414 | O15 | APA | 301 | -21.655 | -10.445 | -0.680  | 1.00 | 19.78 |
| ATOM    | 9415 | C11 | APA | 301 | -21.683 | -11.760 | 1.321   | 1.00 | 19.90 |
| TER     | 9416 |     | APA | 301 |         |         |         |      |       |
| CONNECT | 6    | 5   | 9   |     |         |         |         |      |       |
| CONNECT | 9    | 6   |     |     |         |         |         |      |       |
| CONNECT | 211  | 209 | 210 | 214 |         |         |         |      |       |
| CONNECT | 214  | 211 |     |     |         |         |         |      |       |
| CONNECT | 275  | 273 | 274 | 278 |         |         |         |      |       |
| CONNECT | 278  | 275 |     |     |         |         |         |      |       |
| CONNECT | 330  | 329 | 333 |     |         |         |         |      |       |
| CONNECT | 333  | 330 |     |     |         |         |         |      |       |
| CONNECT | 343  | 341 | 342 | 346 |         |         |         |      |       |
| CONNECT | 346  | 343 |     |     |         |         |         |      |       |
| CONNECT | 429  | 427 | 428 | 432 |         |         |         |      |       |
| CONNECT | 432  | 429 |     |     |         |         |         |      |       |
| CONNECT | 623  | 621 | 622 | 626 |         |         |         |      |       |
| CONNECT | 626  | 623 |     |     |         |         |         |      |       |

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